1,3-Isobenzofurandione, 5-chloro-

Other names: 3-chlorophthalic anhydride
4-chlorophthalic anhydride
Inchi: InChI=1S/C8H3ClO3/c9-4-1-2-5-6(3-4)8(11)12-7(5)10/h1-3H
InchiKey: BTTRMCQEPDPCPA-UHFFFAOYSA-N
Formula: C8H3ClO3
SMILES: O=C1OC(=O)c2cc(Cl)ccc21
Mol. weight [g/mol]: 182.56
CAS: 118-45-6

Physical Properties

Property code	Value	Unit	Source
gf	-165.14	kJ/mol	Joback Method
hf	-324.86	kJ/mol	Joback Method
hfus	18.00	kJ/mol	Joback Method
hvap	54.61	kJ/mol	Joback Method
log10ws	-2.61		Crippen Method
logp	1.651		Crippen Method
mcvol	110.210	ml/mol	McGowan Method
pc	4456.32	kPa	Joback Method
tb	560.00	K	Saturated vapor pressure of 4-fluorophthalic anhydride and 4-chlorophthalic anhydride and isobaric vapor-liquid phase equilibrium of 4-fluorophthalic anhydride + 4-chlorophthalic anhydride: Measurement and modeling
tc	897.36	K	Joback Method
tf	398.70	K	Solubilities of 3-Chlorophthalic Anhydride and 4-Chlorophthalic Anhydride in Different Pure Solvents
vc	0.417	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	245.58	J/mol×K	630.51	Joback Method
cpg	255.69	J/mol×K	674.98	Joback Method
cpg	265.08	J/mol×K	719.46	Joback Method
cpg	273.74	J/mol×K	763.93	Joback Method
cpg	281.65	J/mol×K	808.41	Joback Method
cpg	288.78	J/mol×K	852.88	Joback Method
cpg	295.11	J/mol×K	897.36	Joback Method

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbp	447.27	K	3.41	Saturated vapor pressure of 4-fluorophthalic anhydride and 4-chlorophthalic anhydride and isobaric vapor-liquid phase equilibrium of 4-fluorophthalic anhydride + 4-chlorophthalic anhydride: Measurement and modeling
tbp	454.31	K	4.47	Saturated vapor pressure of 4-fluorophthalic anhydride and 4-chlorophthalic anhydride and isobaric vapor-liquid phase equilibrium of 4-fluorophthalic anhydride + 4-chlorophthalic anhydride: Measurement and modeling

tbp	458.14	K	5.15	Saturated vapor pressure of 4-fluorophthalic anhydride and 4-chlorophthalic anhydride and isobaric vapor-liquid phase equilibrium of 4-fluorophthalic anhydride + 4-chlorophthalic anhydride: Measurement and modeling	
tbp	460.53	K	5.63	Saturated vapor pressure of 4-fluorophthalic anhydride and 4-chlorophthalic anhydride and isobaric vapor-liquid phase equilibrium of 4-fluorophthalic anhydride + 4-chlorophthalic anhydride: Measurement and modeling	
tbp	464.38	K	6.46	Saturated vapor pressure of 4-fluorophthalic anhydride and 4-chlorophthalic anhydride and isobaric vapor-liquid phase equilibrium of 4-fluorophthalic anhydride + 4-chlorophthalic anhydride: Measurement and modeling	
tbp	467.50	K	7.21	Saturated vapor pressure of 4-fluorophthalic anhydride and 4-chlorophthalic anhydride and isobaric vapor-liquid phase equilibrium of 4-fluorophthalic anhydride + 4-chlorophthalic anhydride: Measurement and modeling	

tbp	471.34	K	8.27	Saturated vapor pressure of 4-fluorophthalic anhydride and 4-chlorophthalic anhydride and isobaric vapor-liquid phase equilibrium of 4-fluorophthalic anhydride + 4-chlorophthalic anhydride: Measurement and modeling	
tbp	474.46	K	9.22	Saturated vapor pressure of 4-fluorophthalic anhydride and 4-chlorophthalic anhydride and isobaric vapor-liquid phase equilibrium of 4-fluorophthalic anhydride + 4-chlorophthalic anhydride: Measurement and modeling	
tbp	478.77	K	10.66	Saturated vapor pressure of 4-fluorophthalic anhydride and 4-chlorophthalic anhydride and isobaric vapor-liquid phase equilibrium of 4-fluorophthalic anhydride + 4-chlorophthalic anhydride: Measurement and modeling	
tbp	481.63	K	11.74	Saturated vapor pressure of 4-fluorophthalic anhydride and 4-chlorophthalic anhydride and isobaric vapor-liquid phase equilibrium of 4-fluorophthalic anhydride + 4-chlorophthalic anhydride: Measurement and modeling	

tbp	484.75	K	12.99	Saturated vapor pressure of 4-fluorophthalic anhydride and 4-chlorophthalic anhydride and isobaric vapor-liquid phase equilibrium of 4-fluorophthalic anhydride + 4-chlorophthalic anhydride: Measurement and modeling	
tbp	488.12	K	14.48	Saturated vapor pressure of 4-fluorophthalic anhydride and 4-chlorophthalic anhydride and isobaric vapor-liquid phase equilibrium of 4-fluorophthalic anhydride + 4-chlorophthalic anhydride: Measurement and modeling	
tbp	491.12	K	15.93	Saturated vapor pressure of 4-fluorophthalic anhydride and 4-chlorophthalic anhydride and isobaric vapor-liquid phase equilibrium of 4-fluorophthalic anhydride + 4-chlorophthalic anhydride: Measurement and modeling	
tbp	493.51	K	17.17	Saturated vapor pressure of 4-fluorophthalic anhydride and 4-chlorophthalic anhydride and isobaric vapor-liquid phase equilibrium of 4-fluorophthalic anhydride + 4-chlorophthalic anhydride: Measurement and modeling	

tbp	496.04	K	18.59	Saturated vapor pressure of 4-fluorophthalic anhydride and 4-chlorophthalic anhydride and isobaric vapor-liquid phase equilibrium of 4-fluorophthalic anhydride + 4-chlorophthalic anhydride: Measurement and modeling	
tbp	498.87	K	20.24	Saturated vapor pressure of 4-fluorophthalic anhydride and 4-chlorophthalic anhydride and isobaric vapor-liquid phase equilibrium of 4-fluorophthalic anhydride + 4-chlorophthalic anhydride: Measurement and modeling	
tbp	501.20	K	21.71	Saturated vapor pressure of 4-fluorophthalic anhydride and 4-chlorophthalic anhydride and isobaric vapor-liquid phase equilibrium of 4-fluorophthalic anhydride + 4-chlorophthalic anhydride: Measurement and modeling	
tbp	503.82	K	23.52	Saturated vapor pressure of 4-fluorophthalic anhydride and 4-chlorophthalic anhydride and isobaric vapor-liquid phase equilibrium of 4-fluorophthalic anhydride + 4-chlorophthalic anhydride: Measurement and modeling	

tbp	506.46	K	25.37	Saturated vapor pressure of 4-fluorophthalic anhydride and 4-chlorophthalic anhydride and isobaric vapor-liquid phase equilibrium of 4-fluorophthalic anhydride + 4-chlorophthalic anhydride: Measurement and modeling	
tbp	509.05	K	27.38	Saturated vapor pressure of 4-fluorophthalic anhydride and 4-chlorophthalic anhydride and isobaric vapor-liquid phase equilibrium of 4-fluorophthalic anhydride + 4-chlorophthalic anhydride: Measurement and modeling	
tbp	511.82	K	29.59	Saturated vapor pressure of 4-fluorophthalic anhydride and 4-chlorophthalic anhydride and isobaric vapor-liquid phase equilibrium of 4-fluorophthalic anhydride + 4-chlorophthalic anhydride: Measurement and modeling	
tbp	514.56	K	31.99	Saturated vapor pressure of 4-fluorophthalic anhydride and 4-chlorophthalic anhydride and isobaric vapor-liquid phase equilibrium of 4-fluorophthalic anhydride + 4-chlorophthalic anhydride: Measurement and modeling	

tbp	517.33	K	34.47	Saturated vapor pressure of 4-fluorophthalic anhydride and 4-chlorophthalic anhydride and isobaric vapor-liquid phase equilibrium of 4-fluorophthalic anhydride + 4-chlorophthalic anhydride: Measurement and modeling	
tbp	520.10	K	37.26	Saturated vapor pressure of 4-fluorophthalic anhydride and 4-chlorophthalic anhydride and isobaric vapor-liquid phase equilibrium of 4-fluorophthalic anhydride + 4-chlorophthalic anhydride: Measurement and modeling	
tbp	522.91	K	40.20	Saturated vapor pressure of 4-fluorophthalic anhydride and 4-chlorophthalic anhydride and isobaric vapor-liquid phase equilibrium of 4-fluorophthalic anhydride + 4-chlorophthalic anhydride: Measurement and modeling	
tbp	526.11	K	43.82	Saturated vapor pressure of 4-fluorophthalic anhydride and 4-chlorophthalic anhydride and isobaric vapor-liquid phase equilibrium of 4-fluorophthalic anhydride + 4-chlorophthalic anhydride: Measurement and modeling	

tbp	528.63	K	46.79	Saturated vapor pressure of 4-fluorophthalic anhydride and 4-chlorophthalic anhydride and isobaric vapor-liquid phase equilibrium of 4-fluorophthalic anhydride + 4-chlorophthalic anhydride: Measurement and modeling	
tbp	531.55	K	50.50	Saturated vapor pressure of 4-fluorophthalic anhydride and 4-chlorophthalic anhydride and isobaric vapor-liquid phase equilibrium of 4-fluorophthalic anhydride + 4-chlorophthalic anhydride: Measurement and modeling	
tbp	534.47	K	54.42	Saturated vapor pressure of 4-fluorophthalic anhydride and 4-chlorophthalic anhydride and isobaric vapor-liquid phase equilibrium of 4-fluorophthalic anhydride + 4-chlorophthalic anhydride: Measurement and modeling	
tbp	537.45	K	58.75	Saturated vapor pressure of 4-fluorophthalic anhydride and 4-chlorophthalic anhydride and isobaric vapor-liquid phase equilibrium of 4-fluorophthalic anhydride + 4-chlorophthalic anhydride: Measurement and modeling	

tbp	540.44	K	63.31	Saturated vapor pressure of 4-fluorophthalic anhydride and 4-chlorophthalic anhydride and isobaric vapor-liquid phase equilibrium of 4-fluorophthalic anhydride + 4-chlorophthalic anhydride: Measurement and modeling	
tbp	543.50	K	68.30	Saturated vapor pressure of 4-fluorophthalic anhydride and 4-chlorophthalic anhydride and isobaric vapor-liquid phase equilibrium of 4-fluorophthalic anhydride + 4-chlorophthalic anhydride: Measurement and modeling	
tbp	546.20	K	72.98	Saturated vapor pressure of 4-fluorophthalic anhydride and 4-chlorophthalic anhydride and isobaric vapor-liquid phase equilibrium of 4-fluorophthalic anhydride + 4-chlorophthalic anhydride: Measurement and modeling	
tbp	549.65	K	79.29	Saturated vapor pressure of 4-fluorophthalic anhydride and 4-chlorophthalic anhydride and isobaric vapor-liquid phase equilibrium of 4-fluorophthalic anhydride + 4-chlorophthalic anhydride: Measurement and modeling	

tbp	553.24	K	86.41	Saturated vapor pressure of 4-fluorophthalic anhydride and 4-chlorophthalic anhydride and isobaric vapor-liquid phase equilibrium of 4-fluorophthalic anhydride + 4-chlorophthalic anhydride: Measurement and modeling
tbp	555.97	K	92.12	Saturated vapor pressure of 4-fluorophthalic anhydride and 4-chlorophthalic anhydride and isobaric vapor-liquid phase equilibrium of 4-fluorophthalic anhydride + 4-chlorophthalic anhydride: Measurement and modeling
tbp	559.17	K	99.10	Saturated vapor pressure of 4-fluorophthalic anhydride and 4-chlorophthalic anhydride and isobaric vapor-liquid phase equilibrium of 4-fluorophthalic anhydride + 4-chlorophthalic anhydride: Measurement and modeling

Sources

Solid Liquid Equilibrium and Phase Diagram for the Ternary 4-Chlorophthalic Anhydride + 3-Chlorophthalic Anhydride + Ethyl Acetate System:	https://www.doi.org/10.1021/je3013588
Solubility of 3-Chlorophthalic Anhydride and 4-Chlorophthalic Anhydride in Organic Solvents and Solubility of 3-Chlorophthalic Acid and 4-Chlorophthalic Acid in Water from (283.15 to 333.15) K:	https://www.doi.org/10.1021/je800869g
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
Saturated vapor pressure of 4-fluorophthalic anhydride and 4-chlorophthalic anhydride and isobaric vapor-liquid phase equilibrium of 4-fluorophthalic anhydride + 4-chlorophthalic anhydride: Measurement and modeling:	https://www.doi.org/10.1016/j.fluid.2015.03.030

Measurement and calculation of solid-liquid phase equilibrium for ternary 4-chlorophthalic anhydride + 4-chlorophthalic acid + acetone system:	https://www.doi.org/10.1016/j.fluid.2013.08.032
Solubilities of 3-Chlorophthalic Anhydride and 4-Chlorophthalic Acid (3-Chloro-1(3H)-isobenzofuranone and 4-Chloro-1,3-isobenzofurandione) in Different Pure Solvents:	https://www.doi.org/10.1021/acs.jced.5b00526
NIST Webbook	http://webbook.nist.gov/cgi/cbook.cgi?ID=C118456&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

Legend

cpg:	Ideal gas heat capacity
gf:	Standard Gibbs free energy of formation
hf:	Enthalpy of formation at standard conditions
hfus:	Enthalpy of fusion at standard conditions
hvap:	Enthalpy of vaporization at standard conditions
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
pc:	Critical Pressure
tb:	Normal Boiling Point Temperature
tbp:	Boiling point at given pressure
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume