1,3-Benzenedicarbonyl dichloride

Other names:	1,3-Benzenedicarbonyl chloride
	1,3-Bis(chlorocarbonyl)benzene
	Dichlorid kyseliny isoftalove
	Isophthalic acid chloride
	Isophthalic acid dichloride
	Isophthalic chloride
	Isophthaloyl chloride
	Isophthaloyl dichloride
	Isophthalyl chloride
	Isophthalyl dichloride
	Isothaloyl chloride
	M-BENZENEDICARBONYL CHLORIDE
	M-PHTHALIC DICHLORIDE
	NSC 41884
	m-Phthaloyl chloride
	m-Phthaloyl dichloride
	m-Phthalyl chloride
	m-Phthalyl dichloride
Inchi:	InChI=1S/C8H4Cl2O2/c9-7(11)5-2-1-3-6(4-5)8(10)12/h1-4H
InchiKey:	FDQSRULYDNDXQB-UHFFFAOYSA-N
Formula:	C8H4Cl2O2
SMILES:	O=C(Cl)c1cccc(C(=O)Cl)c1
Mol. weight [g/mol]:	203.02
CAS:	99-63-8

Physical Properties

Property code	Value	Unit	Source
chs	-3400.00 ± 3.00	kJ/mol	NIST Webbook
chs	-3397.70 ± 2.00	kJ/mol	NIST Webbook
gf	-162.44	kJ/mol	Joback Method
hf	-240.03	kJ/mol	Joback Method
hfs	-322.00 ± 2.00	kJ/mol	NIST Webbook
hfs	-365.00	kJ/mol	NIST Webbook
hfus	21.72	kJ/mol	Joback Method
hvap	58.60	kJ/mol	Joback Method
log10ws	-3.25		Crippen Method
logp	2.445		Crippen Method

mcvol	127.440	ml/mol	McGowan Method
pc	3819.82	kPa	Joback Method
tb	549.20	K	NIST Webbook
tc	838.34	K	Joback Method
tf	378.56	K	Joback Method
vc	0.485	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	288.72	J/mol×K	838.34	Joback Method
cpg	283.38	J/mol×K	798.06	Joback Method
cpg	277.47	J/mol×K	757.79	Joback Method
cpg	270.94	J/mol×K	717.52	Joback Method
cpg	263.78	J/mol×K	677.25	Joback Method
cpg	255.95	J/mol×K	636.97	Joback Method
cpg	247.41	J/mol×K	596.70	Joback Method
dvisc	0.0019653	Pa×s	378.56	Joback Method
dvisc	0.0003196	Pa×s	596.70	Joback Method
dvisc	0.0003921	Pa×s	560.34	Joback Method
dvisc	0.0004949	Pa×s	523.99	Joback Method
dvisc	0.0006468	Pa×s	487.63	Joback Method
dvisc	0.0008826	Pa×s	451.27	Joback Method
dvisc	0.0012716	Pa×s	414.92	Joback Method
hvapt	61.50	kJ/mol	496.50	NIST Webbook

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.42901e+01
Coeff. B	-4.59924e+03
Coeff. C	-8.91440e+01
Temperature range (K), min.	417.60
Temperature range (K), max.	601.39

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C99638&Units=SI
The Yaws Handbook of Vapor Pressure:	https://www.sciencedirect.com/book/9780128029992/the-yaws-handbook-of-vapor-pressure
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
KDB:	https://www.cheric.org/files/research/kdb/mol/mol1807.mol
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

Legend

chs:	Standard solid enthalpy of combustion
cpg:	Ideal gas heat capacity
dvisc:	Dynamic viscosity
gf:	Standard Gibbs free energy of formation
hf:	Enthalpy of formation at standard conditions
hfs:	Solid phase enthalpy of formation at standard conditions
hfus:	Enthalpy of fusion at standard conditions
hvap:	Enthalpy of vaporization at standard conditions
hvapt:	Enthalpy of vaporization at a given temperature
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
pc:	Critical Pressure
pvap:	Vapor pressure
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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