3-Fluorophthalic anhydride

Other names: 1,3-Isobenzofurandione, 4-fluoro-
Inchi: InChI=1S/C8H3FO3/c9-5-3-1-2-4-6(5)8(11)12-7(4)10/h1-3H
InchiKey: WWJAZKZLSDRAIV-UHFFFAOYSA-N
Formula: C8H3FO3
SMILES: O=C1OC(=O)c2c(F)cccc21
Mol. weight [g/mol]: 166.11
CAS: 652-39-1

Physical Properties

Property code	Value	Unit	Source
gf	-348.02	kJ/mol	Joback Method
hf	-505.23	kJ/mol	Joback Method
hfus	16.88	kJ/mol	Joback Method
hvap	49.41	kJ/mol	Joback Method
log10ws	-2.26		Crippen Method
logp	1.136		Crippen Method
mcvol	99.740	ml/mol	McGowan Method
pc	4409.10	kPa	Joback Method
tb	592.35	K	Joback Method
tc	842.56	K	Joback Method
tf	417.16	K	Joback Method
vc	0.387	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	233.21	J/mol×K	592.35	Joback Method
cpg	243.52	J/mol×K	634.05	Joback Method
cpg	253.21	J/mol×K	675.75	Joback Method
cpg	262.27	J/mol×K	717.46	Joback Method
cpg	270.66	J/mol×K	759.16	Joback Method
cpg	278.38	J/mol×K	800.86	Joback Method
cpg	285.41	J/mol×K	842.56	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C652391&Units=SI
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

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
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume