3-Fluorophthalic acid

Other names: 1,2-Benzenedicarboxylic acid, 3-fluoro-
Inchi: InChI=1S/C8H5FO4/c9-5-3-1-2-4(7(10)11)6(5)8(12)13/h1-3H,(H,10,11)(H,12,13)
InchiKey: BBCQSMSCEJBIRD-UHFFFAOYSA-N
Formula: C8H5FO4
SMILES: O=C(O)c1cccc(F)c1C(=O)O
Mol. weight [g/mol]: 184.12
CAS: 1583-67-1

Physical Properties

Property code	Value	Unit	Source
gf	-616.66	kJ/mol	Joback Method
hf	-720.59	kJ/mol	Joback Method
hfus	24.19	kJ/mol	Joback Method
hvap	83.03	kJ/mol	Joback Method
log10ws	-1.92		Crippen Method
logp	1.222		Crippen Method
mcvol	116.470	ml/mol	McGowan Method
pc	4959.33	kPa	Joback Method
tb	710.45	K	Joback Method
tc	905.59	K	Joback Method
tf	453.47	K	Joback Method
vc	0.444	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	288.80	J/mol×K	710.45	Joback Method
cpg	294.96	J/mol×K	742.97	Joback Method
cpg	300.70	J/mol×K	775.50	Joback Method
cpg	306.02	J/mol×K	808.02	Joback Method
cpg	310.96	J/mol×K	840.54	Joback Method
cpg	315.51	J/mol×K	873.07	Joback Method
cpg	319.70	J/mol×K	905.59	Joback Method

Sources

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
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C1583671&Units=SI

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