Methyl 2,6-difluorobenzoate

Other names: 2,6-Difluorobenzoic acid, methyl ester
Inchi: InChI=1S/C8H6F2O2/c1-12-8(11)7-5(9)3-2-4-6(7)10/h2-4H,1H3
InchiKey: QNPFLTKQLFSKBY-UHFFFAOYSA-N
Formula: C8H6F2O2
SMILES: COC(=O)c1c(F)cccc1F
Mol. weight [g/mol]: 172.13
CAS: 13671-00-6

Physical Properties

Property code	Value	Unit	Source
gf	-513.91	kJ/mol	Joback Method
hf	-631.88	kJ/mol	Joback Method
hfus	18.69	kJ/mol	Joback Method
hvap	44.52	kJ/mol	Joback Method
log10ws	-2.38		Crippen Method
logp	1.751		Crippen Method
mcvol	110.800	ml/mol	McGowan Method
pc	3345.11	kPa	Joback Method
rinpol	1065.10		NIST Webbook
rinpol	1065.10		NIST Webbook
tb	493.91	K	Joback Method
tc	693.80	K	Joback Method
tf	304.72	K	Joback Method
vc	0.435	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	230.70	J/mol×K	493.91	Joback Method
cpg	240.29	J/mol×K	527.22	Joback Method
cpg	249.43	J/mol×K	560.54	Joback Method
cpg	258.13	J/mol×K	593.85	Joback Method
cpg	266.38	J/mol×K	627.17	Joback Method
cpg	274.20	J/mol×K	660.48	Joback Method

cpg	281.58	J/mol×K	693.80	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=C13671006&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
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume