2,6-Difluorobenzoic acid, 4-methoxyphenyl ester

Inchi: InChI=1S/C14H10F2O3/c1-18-9-5-7-10(8-6-9)19-14(17)13-11(15)3-2-4-12(13)16/h2-8H,1

InchiKey: LTRQIHIOCBEFTR-UHFFFAOYSA-N

Formula: C14H10F2O3

SMILES: COc1ccc(OC(=O)c2c(F)cccc2F)cc1

Mol. weight [g/mol]: 264.22

Physical Properties

Property code	Value	Unit	Source
gf	-465.61	kJ/mol	Joback Method
hf	-662.88	kJ/mol	Joback Method
hfus	29.07	kJ/mol	Joback Method
hvap	63.23	kJ/mol	Joback Method
log10ws	-4.34		Crippen Method
logp	3.193		Crippen Method
mcvol	177.450	ml/mol	McGowan Method
pc	2485.07	kPa	Joback Method
rinpol	1854.00		NIST Webbook
rinpol	1854.00		NIST Webbook
tb	685.27	K	Joback Method
tc	905.92	K	Joback Method
tf	433.51	K	Joback Method
vc	0.681	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	453.84	J/mol×K	685.27	Joback Method
cpg	466.79	J/mol×K	722.04	Joback Method
cpg	478.83	J/mol×K	758.82	Joback Method
cpg	489.96	J/mol×K	795.59	Joback Method
cpg	500.19	J/mol×K	832.37	Joback Method
cpg	509.52	J/mol×K	869.14	Joback Method
cpg	517.97	J/mol×K	905.92	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=U307559&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