2,5-Difluorobenzoic acid, cyclohexyl ester

Inchi: InChI=1S/C13H14F2O2/c14-9-6-7-12(15)11(8-9)13(16)17-10-4-2-1-3-5-10/h6-8,10H,1-5H
InchiKey: NBIGHVXKIHZSDM-UHFFFAOYSA-N
Formula: C13H14F2O2
SMILES: O=C(OC1CCCCC1)c1cc(F)ccc1F
Mol. weight [g/mol]: 240.25

Physical Properties

Property code	Value	Unit	Source
gf	-447.36	kJ/mol	Joback Method
hf	-680.76	kJ/mol	Joback Method
hfus	23.47	kJ/mol	Joback Method
hvap	56.08	kJ/mol	Joback Method
log10ws	-4.48		Crippen Method
logp	3.454		Crippen Method
mcvol	170.390	ml/mol	McGowan Method
pc	2490.03	kPa	Joback Method
rinpol	1621.00		NIST Webbook
rinpol	1621.00		NIST Webbook
tb	627.86	K	Joback Method
tc	847.61	K	Joback Method
tf	368.45	K	Joback Method
vc	0.648	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	449.23	J/mol×K	627.86	Joback Method
cpg	466.12	J/mol×K	664.49	Joback Method
cpg	481.90	J/mol×K	701.11	Joback Method
cpg	496.60	J/mol×K	737.74	Joback Method
cpg	510.23	J/mol×K	774.36	Joback Method
cpg	522.83	J/mol×K	810.99	Joback Method
cpg	534.40	J/mol×K	847.61	Joback Method

Sources

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=U357575&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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