2,5-Difluorobenzoic acid, cyclohexylmethyl ester

Inchi: InChI=1S/C14H16F2O2/c15-11-6-7-13(16)12(8-11)14(17)18-9-10-4-2-1-3-5-10/h6-8,10H

InchiKey: FOIGVDJWDNEQFA-UHFFFAOYSA-N

Formula: C14H16F2O2

SMILES: O=C(OCC1CCCCC1)c1cc(F)ccc1F

Mol. weight [g/mol]: 254.27

Physical Properties

Property code	Value	Unit	Source
gf	-438.94	kJ/mol	Joback Method
hf	-701.40	kJ/mol	Joback Method
hfus	26.06	kJ/mol	Joback Method
hvap	58.31	kJ/mol	Joback Method
log10ws	-4.54		Crippen Method
logp	3.702		Crippen Method
mcvol	184.480	ml/mol	McGowan Method
pc	2267.57	kPa	Joback Method
rinpol	1750.00		NIST Webbook
rinpol	1750.00		NIST Webbook
tb	650.74	K	Joback Method
tc	866.72	K	Joback Method
tf	379.72	K	Joback Method
vc	0.705	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	501.07	J/mol×K	650.74	Joback Method
cpg	518.37	J/mol×K	686.74	Joback Method
cpg	534.54	J/mol×K	722.73	Joback Method
cpg	549.59	J/mol×K	758.73	Joback Method
cpg	563.57	J/mol×K	794.73	Joback Method
cpg	576.48	J/mol×K	830.72	Joback Method
cpg	588.36	J/mol×K	866.72	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=U357578&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