2,6-Difluoro-3-methylbenzoic acid, cyclohexyl ester

Inchi: InChI=1S/C14H16F2O2/c1-9-7-8-11(15)12(13(9)16)14(17)18-10-5-3-2-4-6-10/h7-8,10H,2

InchiKey: ROGZGCASDPRFKV-UHFFFAOYSA-N

Formula: C14H16F2O2

SMILES: Cc1ccc(F)c(C(=O)OC2CCCCC2)c1F

Mol. weight [g/mol]: 254.27

Physical Properties

Property code	Value	Unit	Source
gf	-448.57	kJ/mol	Joback Method
hf	-712.87	kJ/mol	Joback Method
hfus	25.67	kJ/mol	Joback Method
hvap	58.97	kJ/mol	Joback Method
log10ws	-4.95		Crippen Method
logp	3.763		Crippen Method
mcvol	184.480	ml/mol	McGowan Method
pc	2235.52	kPa	Joback Method
rinpol	1759.00		NIST Webbook
tb	655.72	K	Joback Method
tc	872.58	K	Joback Method
tf	392.24	K	Joback Method
vc	0.705	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	500.63	J/mol×K	655.72	Joback Method
cpg	517.73	J/mol×K	691.86	Joback Method
cpg	533.73	J/mol×K	728.01	Joback Method
cpg	548.65	J/mol×K	764.15	Joback Method
cpg	562.50	J/mol×K	800.29	Joback Method
cpg	575.31	J/mol×K	836.43	Joback Method
cpg	587.09	J/mol×K	872.58	Joback Method

Sources

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=U357677&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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