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

Inchi: InChI=1S/C14H18F2O2/c1-9(2)5-4-8-18-14(17)12-11(15)7-6-10(3)13(12)16/h6-7,9H,4-5,

InchiKey: KVYAEZHJDUTLNF-UHFFFAOYSA-N

Formula: C14H18F2O2

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

Mol. weight [g/mol]: 256.29

Physical Properties

Property code	Value	Unit	Source
gf	-475.46	kJ/mol	Joback Method
hf	-772.47	kJ/mol	Joback Method
hfus	30.31	kJ/mol	Joback Method
hvap	58.15	kJ/mol	Joback Method
log10ws	-4.70		Crippen Method
logp	3.866		Crippen Method
mcvol	195.340	ml/mol	McGowan Method
pc	1870.79	kPa	Joback Method
rinpol	1642.00		NIST Webbook
rinpol	1642.00		NIST Webbook
tb	635.73	K	Joback Method
tc	825.69	K	Joback Method
tf	369.86	K	Joback Method
vc	0.765	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	509.62	J/mol×K	635.73	Joback Method
cpg	524.32	J/mol×K	667.39	Joback Method
cpg	538.29	J/mol×K	699.05	Joback Method
cpg	551.53	J/mol×K	730.71	Joback Method
cpg	564.05	J/mol×K	762.37	Joback Method
cpg	575.86	J/mol×K	794.03	Joback Method
cpg	586.98	J/mol×K	825.69	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U338842&Units=SI
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

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