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

Inchi: InChI=1S/C14H18F2O2/c1-3-4-5-6-9-18-14(17)12-11(15)8-7-10(2)13(12)16/h7-8H,3-6,9H
InchiKey: WJOFANTVFUDTHO-UHFFFAOYSA-N
Formula: C14H18F2O2
SMILES: CCCCCCOC(=O)c1c(F)ccc(C)c1F
Mol. weight [g/mol]: 256.29

Physical Properties

Property code	Value	Unit	Source
gf	-473.02	kJ/mol	Joback Method
hf	-767.19	kJ/mol	Joback Method
hfus	33.84	kJ/mol	Joback Method
hvap	58.54	kJ/mol	Joback Method
log10ws	-4.95		Crippen Method
logp	4.010		Crippen Method
mcvol	195.340	ml/mol	McGowan Method
pc	1857.91	kPa	Joback Method
rinpol	1698.00		NIST Webbook
rinpol	1698.00		NIST Webbook
tb	636.17	K	Joback Method
tc	822.94	K	Joback Method
tf	384.86	K	Joback Method
vc	0.771	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	509.17	J/mol×K	636.17	Joback Method
cpg	523.59	J/mol×K	667.30	Joback Method
cpg	537.30	J/mol×K	698.43	Joback Method
cpg	550.32	J/mol×K	729.56	Joback Method
cpg	562.65	J/mol×K	760.69	Joback Method
cpg	574.31	J/mol×K	791.82	Joback Method
cpg	585.30	J/mol×K	822.94	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U338843&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

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