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

Inchi: InChI=1S/C16H22F2O2/c1-3-4-5-6-7-8-11-20-16(19)14-13(17)10-9-12(2)15(14)18/h9-10
InchiKey: SKKAAXWBGOWBDI-UHFFFAOYSA-N
Formula: C16H22F2O2
SMILES: CCCCCCCCOC(=O)c1c(F)ccc(C)c1F
Mol. weight [g/mol]: 284.34

Physical Properties

Property code	Value	Unit	Source
gf	-456.18	kJ/mol	Joback Method
hf	-808.47	kJ/mol	Joback Method
hfus	39.02	kJ/mol	Joback Method
hvap	62.99	kJ/mol	Joback Method
log10ws	-5.78		Crippen Method
logp	4.791		Crippen Method
mcvol	223.520	ml/mol	McGowan Method
pc	1584.75	kPa	Joback Method
rinpol	1896.00		NIST Webbook
rinpol	1896.00		NIST Webbook
tb	681.93	K	Joback Method
tc	866.02	K	Joback Method
tf	407.40	K	Joback Method
vc	0.883	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	614.82	J/mol×K	681.93	Joback Method
cpg	630.26	J/mol×K	712.61	Joback Method
cpg	644.92	J/mol×K	743.29	Joback Method
cpg	658.81	J/mol×K	773.98	Joback Method
cpg	671.94	J/mol×K	804.66	Joback Method
cpg	684.34	J/mol×K	835.34	Joback Method
cpg	696.01	J/mol×K	866.02	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=U338845&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