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

Inchi: InChI=1S/C19H28F2O2/c1-3-4-5-6-7-8-9-10-11-14-23-19(22)17-16(20)13-12-15(2)18(17
InchiKey: KPKUYQIHBFLCNN-UHFFFAOYSA-N
Formula: C19H28F2O2
SMILES: CCCCCCCCCCCOC(=O)c1c(F)ccc(C)c1F
Mol. weight [g/mol]: 326.42

Physical Properties

Property code	Value	Unit	Source
gf	-430.92	kJ/mol	Joback Method
hf	-870.39	kJ/mol	Joback Method
hfus	46.79	kJ/mol	Joback Method
hvap	69.67	kJ/mol	Joback Method
log10ws	-7.04		Crippen Method
logp	5.961		Crippen Method
mcvol	265.790	ml/mol	McGowan Method
pc	1275.51	kPa	Joback Method
rinpol	2198.00		NIST Webbook
rinpol	2198.00		NIST Webbook
tb	750.57	K	Joback Method
tc	933.95	K	Joback Method
tf	441.21	K	Joback Method
vc	1.052	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	782.62	J/mol×K	750.57	Joback Method
cpg	799.27	J/mol×K	781.13	Joback Method
cpg	815.03	J/mol×K	811.70	Joback Method
cpg	829.91	J/mol×K	842.26	Joback Method
cpg	843.94	J/mol×K	872.82	Joback Method
cpg	857.13	J/mol×K	903.39	Joback Method
cpg	869.51	J/mol×K	933.95	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U338848&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