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

Inchi: InChI=1S/C25H40F2O2/c1-3-4-5-6-7-8-9-10-11-12-13-14-15-16-17-20-29-25(28)23-22(2

InchiKey: TUIJKTFSLGICPS-UHFFFAOYSA-N

Formula: C25H40F2O2

SMILES: CCCCCCCCCCCCCCCCCOC(=O)c1c(F)ccc(C)c1F

Mol. weight [g/mol]: 410.58

Physical Properties

Property code	Value	Unit	Source
gf	-380.40	kJ/mol	Joback Method
hf	-994.23	kJ/mol	Joback Method
hfus	62.33	kJ/mol	Joback Method
hvap	83.03	kJ/mol	Joback Method
log10ws	-9.55		Crippen Method
logp	8.301		Crippen Method
mcvol	350.330	ml/mol	McGowan Method
pc	877.39	kPa	Joback Method
rinpol	2814.00		NIST Webbook
rinpol	2814.00		NIST Webbook
tb	887.85	K	Joback Method
tc	1086.98	K	Joback Method
tf	508.83	K	Joback Method
vc	1.387	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1143.83	J/mol×K	887.85	Joback Method
cpg	1162.82	J/mol×K	921.04	Joback Method
cpg	1180.57	J/mol×K	954.23	Joback Method
cpg	1197.14	J/mol×K	987.41	Joback Method
cpg	1212.55	J/mol×K	1020.60	Joback Method
cpg	1226.85	J/mol×K	1053.79	Joback Method
cpg	1240.08	J/mol×K	1086.98	Joback Method

Sources

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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U338854&Units=SI

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