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

Inchi: InChI=1S/C26H42F2O2/c1-3-4-5-6-7-8-9-10-11-12-13-14-15-16-17-18-21-30-26(29)24-2

InchiKey: GUWSMFDAWJODSP-UHFFFAOYSA-N

Formula: C26H42F2O2

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

Mol. weight [g/mol]: 424.61

Physical Properties

Property code	Value	Unit	Source
gf	-371.98	kJ/mol	Joback Method
hf	-1014.87	kJ/mol	Joback Method
hfus	64.92	kJ/mol	Joback Method
hvap	85.25	kJ/mol	Joback Method
log10ws	-9.97		Crippen Method
logp	8.692		Crippen Method
mcvol	364.420	ml/mol	McGowan Method
pc	829.55	kPa	Joback Method
rinpol	2921.00		NIST Webbook
rinpol	2921.00		NIST Webbook
tb	910.73	K	Joback Method
tc	1115.41	K	Joback Method
tf	520.10	K	Joback Method
vc	1.444	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1206.53	J/mol×K	910.73	Joback Method
cpg	1226.00	J/mol×K	944.84	Joback Method
cpg	1244.15	J/mol×K	978.96	Joback Method
cpg	1261.03	J/mol×K	1013.07	Joback Method
cpg	1276.67	J/mol×K	1047.18	Joback Method
cpg	1291.14	J/mol×K	1081.30	Joback Method
cpg	1304.48	J/mol×K	1115.41	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=U338855&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