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

Inchi: InChI=1S/C24H38F2O2/c1-3-4-5-6-7-8-9-10-11-12-13-14-15-16-19-28-24(27)22-21(25)1

InchiKey: JDAQLVSRLALOEM-UHFFFAOYSA-N

Formula: C24H38F2O2

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

Mol. weight [g/mol]: 396.55

Physical Properties

Property code	Value	Unit	Source
gf	-388.82	kJ/mol	Joback Method
hf	-973.59	kJ/mol	Joback Method
hfus	59.74	kJ/mol	Joback Method
hvap	80.80	kJ/mol	Joback Method
log10ws	-9.13		Crippen Method
logp	7.911		Crippen Method
mcvol	336.240	ml/mol	McGowan Method
pc	929.51	kPa	Joback Method
rinpol	2728.00		NIST Webbook
rinpol	2728.00		NIST Webbook
tb	864.97	K	Joback Method
tc	1059.50	K	Joback Method
tf	497.56	K	Joback Method
vc	1.331	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1081.73	J/mol×K	864.97	Joback Method
cpg	1100.28	J/mol×K	897.39	Joback Method
cpg	1117.67	J/mol×K	929.81	Joback Method
cpg	1133.94	J/mol×K	962.23	Joback Method
cpg	1149.12	J/mol×K	994.65	Joback Method
cpg	1163.25	J/mol×K	1027.07	Joback Method
cpg	1176.37	J/mol×K	1059.50	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=U338853&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