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

Inchi: InChI=1S/C23H36F2O2/c1-3-4-5-6-7-8-9-10-11-12-13-14-15-18-27-23(26)21-20(24)17-1
InchiKey: GDUDFOFZZXIORV-UHFFFAOYSA-N
Formula: C23H36F2O2
SMILES: CCCCCCCCCCCCCCCOC(=O)c1c(F)ccc(C)c1F
Mol. weight [g/mol]: 382.53

Physical Properties

Property code	Value	Unit	Source
gf	-397.24	kJ/mol	Joback Method
hf	-952.95	kJ/mol	Joback Method
hfus	57.15	kJ/mol	Joback Method
hvap	78.58	kJ/mol	Joback Method
log10ws	-8.71		Crippen Method
logp	7.521		Crippen Method
mcvol	322.150	ml/mol	McGowan Method
pc	986.40	kPa	Joback Method
rinpol	2634.00		NIST Webbook
rinpol	2634.00		NIST Webbook
tb	842.09	K	Joback Method
tc	1032.89	K	Joback Method
tf	486.29	K	Joback Method
vc	1.276	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1020.31	J/mol×K	842.09	Joback Method
cpg	1038.45	J/mol×K	873.89	Joback Method
cpg	1055.49	J/mol×K	905.69	Joback Method
cpg	1071.48	J/mol×K	937.49	Joback Method
cpg	1086.44	J/mol×K	969.29	Joback Method
cpg	1100.40	J/mol×K	1001.09	Joback Method
cpg	1113.39	J/mol×K	1032.89	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U338852&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

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