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

Inchi: InChI=1S/C22H34F2O2/c1-4-6-7-8-9-10-11-12-13-14-18(5-2)26-22(25)20-19(23)16-15-1

InchiKey: ZGWVVEPPWDVOJV-UHFFFAOYSA-N

Formula: C22H34F2O2

SMILES: CCCCCCCCCCCC(CC)OC(=O)c1c(F)ccc(C)c1F

Mol. weight [g/mol]: 368.50

Physical Properties

Property code	Value	Unit	Source
gf	-408.10	kJ/mol	Joback Method
hf	-937.59	kJ/mol	Joback Method
hfus	51.03	kJ/mol	Joback Method
hvap	75.96	kJ/mol	Joback Method
log10ws	-8.41		Crippen Method
logp	7.130		Crippen Method
mcvol	308.060	ml/mol	McGowan Method
pc	1054.14	kPa	Joback Method
rinpol	2416.00		NIST Webbook
rinpol	2416.00		NIST Webbook
tb	818.77	K	Joback Method
tc	1007.66	K	Joback Method
tf	460.02	K	Joback Method
vc	1.214	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	960.11	J/mol×K	818.77	Joback Method
cpg	977.95	J/mol×K	850.25	Joback Method
cpg	994.74	J/mol×K	881.73	Joback Method
cpg	1010.50	J/mol×K	913.22	Joback Method
cpg	1025.27	J/mol×K	944.70	Joback Method
cpg	1039.07	J/mol×K	976.18	Joback Method
cpg	1051.93	J/mol×K	1007.66	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U338587&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