2,6-Difluoro-3-methylbenzoic acid, 4-pentadecyl ester

Inchi: InChI=1S/C23H36F2O2/c1-4-6-7-8-9-10-11-12-13-15-19(14-5-2)27-23(26)21-20(24)17-1

InchiKey: ZTYUQUHSGCBOME-UHFFFAOYSA-N

Formula: C23H36F2O2

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

Mol. weight [g/mol]: 382.53

Physical Properties

Property code	Value	Unit	Source
gf	-399.68	kJ/mol	Joback Method
hf	-958.23	kJ/mol	Joback Method
hfus	53.62	kJ/mol	Joback Method
hvap	78.19	kJ/mol	Joback Method
log10ws	-8.83		Crippen Method
logp	7.520		Crippen Method
mcvol	322.150	ml/mol	McGowan Method
pc	991.38	kPa	Joback Method
rinpol	2491.00		NIST Webbook
rinpol	2491.00		NIST Webbook
tb	841.65	K	Joback Method
tc	1033.14	K	Joback Method
tf	471.29	K	Joback Method
vc	1.270	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1020.79	J/mol×K	841.65	Joback Method
cpg	1038.98	J/mol×K	873.56	Joback Method
cpg	1056.07	J/mol×K	905.48	Joback Method
cpg	1072.08	J/mol×K	937.39	Joback Method
cpg	1087.04	J/mol×K	969.31	Joback Method
cpg	1100.99	J/mol×K	1001.22	Joback Method
cpg	1113.95	J/mol×K	1033.14	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=U338592&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