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

Inchi: InChI=1S/C21H32F2O2/c1-4-5-6-7-8-9-10-11-12-13-17(3)25-21(24)19-18(22)15-14-16(2

InchiKey: XRKJJYZSEWPTPO-UHFFFAOYSA-N

Formula: C21H32F2O2

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

Mol. weight [g/mol]: 354.47

Physical Properties

Property code	Value	Unit	Source
gf	-416.52	kJ/mol	Joback Method
hf	-916.95	kJ/mol	Joback Method
hfus	48.44	kJ/mol	Joback Method
hvap	73.74	kJ/mol	Joback Method
log10ws	-7.99		Crippen Method
logp	6.739		Crippen Method
mcvol	293.970	ml/mol	McGowan Method
pc	1123.06	kPa	Joback Method
rinpol	2330.00		NIST Webbook
rinpol	2330.00		NIST Webbook
tb	795.89	K	Joback Method
tc	982.92	K	Joback Method
tf	448.75	K	Joback Method
vc	1.157	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	900.22	J/mol×K	795.89	Joback Method
cpg	917.73	J/mol×K	827.06	Joback Method
cpg	934.23	J/mol×K	858.23	Joback Method
cpg	949.75	J/mol×K	889.41	Joback Method
cpg	964.32	J/mol×K	920.58	Joback Method
cpg	977.96	J/mol×K	951.75	Joback Method
cpg	990.69	J/mol×K	982.92	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=U338582&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