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

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

InchiKey: RZCDMHNCZOSTSL-UHFFFAOYSA-N

Formula: C21H32F2O2

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

Mol. weight [g/mol]: 354.47

Physical Properties

Property code	Value	Unit	Source
gf	-414.08	kJ/mol	Joback Method
hf	-911.67	kJ/mol	Joback Method
hfus	51.97	kJ/mol	Joback Method
hvap	74.12	kJ/mol	Joback Method
log10ws	-7.88		Crippen Method
logp	6.741		Crippen Method
mcvol	293.970	ml/mol	McGowan Method
pc	1117.06	kPa	Joback Method
rinpol	2412.00		NIST Webbook
rinpol	2412.00		NIST Webbook
tb	796.33	K	Joback Method
tc	982.04	K	Joback Method
tf	463.75	K	Joback Method
vc	1.163	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	899.72	J/mol×K	796.33	Joback Method
cpg	917.10	J/mol×K	827.28	Joback Method
cpg	933.50	J/mol×K	858.23	Joback Method
cpg	948.94	J/mol×K	889.19	Joback Method
cpg	963.45	J/mol×K	920.14	Joback Method
cpg	977.05	J/mol×K	951.09	Joback Method
cpg	989.77	J/mol×K	982.04	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=U338850&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