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

Inchi: InChI=1S/C17H24F2O2/c1-3-4-5-6-7-8-9-12-21-17(20)15-14(18)11-10-13(2)16(15)19/h1
InchiKey: ZIWQGGZBEOHRAL-UHFFFAOYSA-N
Formula: C17H24F2O2
SMILES: CCCCCCCCCOC(=O)c1c(F)ccc(C)c1F
Mol. weight [g/mol]: 298.37

Physical Properties

Property code	Value	Unit	Source
gf	-447.76	kJ/mol	Joback Method
hf	-829.11	kJ/mol	Joback Method
hfus	41.61	kJ/mol	Joback Method
hvap	65.22	kJ/mol	Joback Method
log10ws	-6.20		Crippen Method
logp	5.181		Crippen Method
mcvol	237.610	ml/mol	McGowan Method
pc	1470.23	kPa	Joback Method
rinpol	2002.00		NIST Webbook
rinpol	2002.00		NIST Webbook
tb	704.81	K	Joback Method
tc	888.17	K	Joback Method
tf	418.67	K	Joback Method
vc	0.940	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	669.60	J/mol×K	704.81	Joback Method
cpg	685.47	J/mol×K	735.37	Joback Method
cpg	700.53	J/mol×K	765.93	Joback Method
cpg	714.78	J/mol×K	796.49	Joback Method
cpg	728.25	J/mol×K	827.05	Joback Method
cpg	740.95	J/mol×K	857.61	Joback Method
cpg	752.89	J/mol×K	888.17	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=U338846&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