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

Inchi: InChI=1S/C27H44F2O2/c1-3-4-5-6-7-8-9-10-11-12-13-14-15-16-17-18-19-22-31-27(30)2
InchiKey: GZCRDPVIDCKTAD-UHFFFAOYSA-N
Formula: C27H44F2O2
SMILES: CCCCCCCCCCCCCCCCCCCOC(=O)c1c(F)ccc(C)c1F
Mol. weight [g/mol]: 438.63

Physical Properties

Property code	Value	Unit	Source
gf	-363.56	kJ/mol	Joback Method
hf	-1035.51	kJ/mol	Joback Method
hfus	67.51	kJ/mol	Joback Method
hvap	87.48	kJ/mol	Joback Method
log10ws	-10.39		Crippen Method
logp	9.082		Crippen Method
mcvol	378.510	ml/mol	McGowan Method
pc	785.51	kPa	Joback Method
rinpol	3048.00		NIST Webbook
rinpol	3048.00		NIST Webbook
tb	933.61	K	Joback Method
tc	1144.87	K	Joback Method
tf	531.37	K	Joback Method
vc	1.500	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1269.79	J/mol×K	933.61	Joback Method
cpg	1289.78	J/mol×K	968.82	Joback Method
cpg	1308.35	J/mol×K	1004.03	Joback Method
cpg	1325.56	J/mol×K	1039.24	Joback Method
cpg	1341.45	J/mol×K	1074.45	Joback Method
cpg	1356.09	J/mol×K	1109.66	Joback Method
cpg	1369.53	J/mol×K	1144.87	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U338856&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

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