2,5-Difluorobenzoic acid, nonyl ester

Inchi: InChI=1S/C16H22F2O2/c1-2-3-4-5-6-7-8-11-20-16(19)14-12-13(17)9-10-15(14)18/h9-10
InchiKey: IUVDQGJNSQVPAZ-UHFFFAOYSA-N
Formula: C16H22F2O2
SMILES: CCCCCCCCCOC(=O)c1cc(F)ccc1F
Mol. weight [g/mol]: 284.34

Physical Properties

Property code	Value	Unit	Source
gf	-446.55	kJ/mol	Joback Method
hf	-797.00	kJ/mol	Joback Method
hfus	39.41	kJ/mol	Joback Method
hvap	62.33	kJ/mol	Joback Method
log10ws	-5.73		Crippen Method
logp	4.872		Crippen Method
mcvol	223.520	ml/mol	McGowan Method
pc	1603.85	kPa	Joback Method
rinpol	1880.00		NIST Webbook
rinpol	1880.00		NIST Webbook
tb	676.95	K	Joback Method
tc	860.19	K	Joback Method
tf	394.88	K	Joback Method
vc	0.883	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	615.21	J/mol×K	676.95	Joback Method
cpg	630.78	J/mol×K	707.49	Joback Method
cpg	645.55	J/mol×K	738.03	Joback Method
cpg	659.53	J/mol×K	768.57	Joback Method
cpg	672.75	J/mol×K	799.11	Joback Method
cpg	685.22	J/mol×K	829.65	Joback Method
cpg	696.96	J/mol×K	860.19	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=U338808&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