2,5-Difluorobenzoic acid, eicosyl ester

Inchi: InChI=1S/C27H44F2O2/c1-2-3-4-5-6-7-8-9-10-11-12-13-14-15-16-17-18-19-22-31-27(30
InchiKey: KGZAQRYPXQTLRV-UHFFFAOYSA-N
Formula: C27H44F2O2
SMILES: CCCCCCCCCCCCCCCCCCCCOC(=O)c1cc(F)ccc1F
Mol. weight [g/mol]: 438.63

Physical Properties

Property code	Value	Unit	Source
gf	-353.93	kJ/mol	Joback Method
hf	-1024.04	kJ/mol	Joback Method
hfus	67.90	kJ/mol	Joback Method
hvap	86.82	kJ/mol	Joback Method
log10ws	-10.33		Crippen Method
logp	9.163		Crippen Method
mcvol	378.510	ml/mol	McGowan Method
pc	792.15	kPa	Joback Method
rinpol	2976.00		NIST Webbook
rinpol	2976.00		NIST Webbook
tb	928.63	K	Joback Method
tc	1138.63	K	Joback Method
tf	518.85	K	Joback Method
vc	1.500	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1269.91	J/mol×K	928.63	Joback Method
cpg	1289.97	J/mol×K	963.63	Joback Method
cpg	1308.64	J/mol×K	998.63	Joback Method
cpg	1325.96	J/mol×K	1033.63	Joback Method
cpg	1342.01	J/mol×K	1068.63	Joback Method
cpg	1356.83	J/mol×K	1103.63	Joback Method
cpg	1370.50	J/mol×K	1138.63	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U338818&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

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