3,4-Difluorobenzoic acid, octadecyl ester

Inchi: InChI=1S/C25H40F2O2/c1-2-3-4-5-6-7-8-9-10-11-12-13-14-15-16-17-20-29-25(28)22-18
InchiKey: CZBMODSKJUZROH-UHFFFAOYSA-N
Formula: C25H40F2O2
SMILES: CCCCCCCCCCCCCCCCCCCCOC(=O)c1ccc(F)c(F)c1
Mol. weight [g/mol]: 410.58

Physical Properties

Property code	Value	Unit	Source
gf	-370.77	kJ/mol	Joback Method
hf	-982.76	kJ/mol	Joback Method
hfus	62.72	kJ/mol	Joback Method
hvap	82.37	kJ/mol	Joback Method
log10ws	-9.49		Crippen Method
logp	8.383		Crippen Method
mcvol	350.330	ml/mol	McGowan Method
pc	885.24	kPa	Joback Method
rinpol	2770.00		NIST Webbook
rinpol	2770.00		NIST Webbook
tb	882.87	K	Joback Method
tc	1080.89	K	Joback Method
tf	496.31	K	Joback Method
vc	1.387	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1143.96	J/mol×K	882.87	Joback Method
cpg	1163.02	J/mol×K	915.87	Joback Method
cpg	1180.85	J/mol×K	948.88	Joback Method
cpg	1197.50	J/mol×K	981.88	Joback Method
cpg	1213.02	J/mol×K	1014.88	Joback Method
cpg	1227.45	J/mol×K	1047.89	Joback Method
cpg	1240.84	J/mol×K	1080.89	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=U338874&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