3,4-Difluorobenzoic acid, pentadecyl ester

Inchi: InChI=1S/C22H34F2O2/c1-2-3-4-5-6-7-8-9-10-11-12-13-14-17-26-22(25)19-15-16-20(23
InchiKey: DOZMTPZUTLUQQI-UHFFFAOYSA-N
Formula: C22H34F2O2
SMILES: CCCCCCCCCCCCCCCOC(=O)c1ccc(F)c(F)c1
Mol. weight [g/mol]: 368.50

Physical Properties

Property code	Value	Unit	Source
gf	-396.03	kJ/mol	Joback Method
hf	-920.84	kJ/mol	Joback Method
hfus	54.95	kJ/mol	Joback Method
hvap	75.69	kJ/mol	Joback Method
log10ws	-8.24		Crippen Method
logp	7.213		Crippen Method
mcvol	308.060	ml/mol	McGowan Method
pc	1058.95	kPa	Joback Method
rinpol	2474.00		NIST Webbook
rinpol	2474.00		NIST Webbook
tb	814.23	K	Joback Method
tc	1001.16	K	Joback Method
tf	462.50	K	Joback Method
vc	1.220	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	959.82	J/mol×K	814.23	Joback Method
cpg	977.64	J/mol×K	845.38	Joback Method
cpg	994.43	J/mol×K	876.54	Joback Method
cpg	1010.21	J/mol×K	907.69	Joback Method
cpg	1025.02	J/mol×K	938.85	Joback Method
cpg	1038.89	J/mol×K	970.00	Joback Method
cpg	1051.85	J/mol×K	1001.16	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U338871&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