2,4-Difluorobenzoic acid, hexadecyl ester

Inchi: InChI=1S/C23H36F2O2/c1-2-3-4-5-6-7-8-9-10-11-12-13-14-15-18-27-23(26)21-17-16-20
InchiKey: CSUMTYMCGJBOPG-UHFFFAOYSA-N
Formula: C23H36F2O2
SMILES: CCCCCCCCCCCCCCCCOC(=O)c1ccc(F)cc1F
Mol. weight [g/mol]: 382.53

Physical Properties

Property code	Value	Unit	Source
gf	-387.61	kJ/mol	Joback Method
hf	-941.48	kJ/mol	Joback Method
hfus	57.54	kJ/mol	Joback Method
hvap	77.91	kJ/mol	Joback Method
log10ws	-8.66		Crippen Method
logp	7.603		Crippen Method
mcvol	322.150	ml/mol	McGowan Method
pc	995.76	kPa	Joback Method
rinpol	2796.00		NIST Webbook
rinpol	2796.00		NIST Webbook
tb	837.11	K	Joback Method
tc	1026.91	K	Joback Method
tf	473.77	K	Joback Method
vc	1.276	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1020.49	J/mol×K	837.11	Joback Method
cpg	1038.69	J/mol×K	868.74	Joback Method
cpg	1055.80	J/mol×K	900.38	Joback Method
cpg	1071.86	J/mol×K	932.01	Joback Method
cpg	1086.90	J/mol×K	963.64	Joback Method
cpg	1100.96	J/mol×K	995.28	Joback Method
cpg	1114.07	J/mol×K	1026.91	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=U338794&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

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