2,4-Difluorobenzoic acid, heptadecyl ester

Inchi: InChI=1S/C24H38F2O2/c1-2-3-4-5-6-7-8-9-10-11-12-13-14-15-16-19-28-24(27)22-18-17
InchiKey: SOEYMVOIKNZTDI-UHFFFAOYSA-N
Formula: C24H38F2O2
SMILES: CCCCCCCCCCCCCCCCCOC(=O)c1ccc(F)cc1F
Mol. weight [g/mol]: 396.55

Physical Properties

Property code	Value	Unit	Source
gf	-379.19	kJ/mol	Joback Method
hf	-962.12	kJ/mol	Joback Method
hfus	60.13	kJ/mol	Joback Method
hvap	80.14	kJ/mol	Joback Method
log10ws	-9.07		Crippen Method
logp	7.993		Crippen Method
mcvol	336.240	ml/mol	McGowan Method
pc	938.07	kPa	Joback Method
rinpol	2699.00		NIST Webbook
rinpol	2699.00		NIST Webbook
tb	859.99	K	Joback Method
tc	1053.47	K	Joback Method
tf	485.04	K	Joback Method
vc	1.331	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1081.89	J/mol×K	859.99	Joback Method
cpg	1100.50	J/mol×K	892.24	Joback Method
cpg	1117.96	J/mol×K	924.48	Joback Method
cpg	1134.31	J/mol×K	956.73	Joback Method
cpg	1149.58	J/mol×K	988.97	Joback Method
cpg	1163.83	J/mol×K	1021.22	Joback Method
cpg	1177.08	J/mol×K	1053.47	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=U338795&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