3,4-Difluorobenzoic acid, tetradecyl ester

Inchi: InChI=1S/C21H32F2O2/c1-2-3-4-5-6-7-8-9-10-11-12-13-16-25-21(24)18-14-15-19(22)20
InchiKey: HNFNBFHQNDOKQO-UHFFFAOYSA-N
Formula: C21H32F2O2
SMILES: CCCCCCCCCCCCCCOC(=O)c1ccc(F)c(F)c1
Mol. weight [g/mol]: 354.47

Physical Properties

Property code	Value	Unit	Source
gf	-404.45	kJ/mol	Joback Method
hf	-900.20	kJ/mol	Joback Method
hfus	52.36	kJ/mol	Joback Method
hvap	73.46	kJ/mol	Joback Method
log10ws	-7.82		Crippen Method
logp	6.823		Crippen Method
mcvol	293.970	ml/mol	McGowan Method
pc	1128.35	kPa	Joback Method
rinpol	2364.00		NIST Webbook
rinpol	2364.00		NIST Webbook
tb	791.35	K	Joback Method
tc	976.14	K	Joback Method
tf	451.23	K	Joback Method
vc	1.163	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	899.96	J/mol×K	791.35	Joback Method
cpg	917.42	J/mol×K	822.15	Joback Method
cpg	933.88	J/mol×K	852.95	Joback Method
cpg	949.39	J/mol×K	883.75	Joback Method
cpg	963.97	J/mol×K	914.55	Joback Method
cpg	977.65	J/mol×K	945.34	Joback Method
cpg	990.46	J/mol×K	976.14	Joback Method

Sources

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=U338870&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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