2,5-Difluorobenzoic acid, 3-tetradecyl ester

Inchi: InChI=1S/C21H32F2O2/c1-3-5-6-7-8-9-10-11-12-13-18(4-2)25-21(24)19-16-17(22)14-15
InchiKey: BTTPADYCZYPHKB-UHFFFAOYSA-N
Formula: C21H32F2O2
SMILES: CCCCCCCCCCCC(CC)OC(=O)c1cc(F)ccc1F
Mol. weight [g/mol]: 354.47

Physical Properties

Property code	Value	Unit	Source
gf	-406.89	kJ/mol	Joback Method
hf	-905.48	kJ/mol	Joback Method
hfus	48.83	kJ/mol	Joback Method
hvap	73.07	kJ/mol	Joback Method
log10ws	-7.93		Crippen Method
logp	6.821		Crippen Method
mcvol	293.970	ml/mol	McGowan Method
pc	1134.43	kPa	Joback Method
rinpol	2242.00		NIST Webbook
rinpol	2242.00		NIST Webbook
tb	790.91	K	Joback Method
tc	977.04	K	Joback Method
tf	436.23	K	Joback Method
vc	1.157	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	900.46	J/mol×K	790.91	Joback Method
cpg	918.04	J/mol×K	821.93	Joback Method
cpg	934.61	J/mol×K	852.95	Joback Method
cpg	950.21	J/mol×K	883.98	Joback Method
cpg	964.85	J/mol×K	915.00	Joback Method
cpg	978.57	J/mol×K	946.02	Joback Method
cpg	991.40	J/mol×K	977.04	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U338479&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

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