Phthalic acid, 2,5-difluorobenzyl heptadecyl ester

Inchi: InChI=1S/C32H44F2O4/c1-2-3-4-5-6-7-8-9-10-11-12-13-14-15-18-23-37-31(35)28-19-16
InchiKey: SEQONKMVPKKERO-UHFFFAOYSA-N
Formula: C32H44F2O4
SMILES: CCCCCCCCCCCCCCCCCOC(=O)c1ccccc1C(=O)OCc1cc(F)ccc1F
Mol. weight [g/mol]: 530.69

Physical Properties

Property code	Value	Unit	Source
gf	-442.97	kJ/mol	Joback Method
hf	-1146.98	kJ/mol	Joback Method
hfus	77.28	kJ/mol	Joback Method
hvap	110.04	kJ/mol	Joback Method
log10ws	-11.43		Crippen Method
logp	9.350		Crippen Method
mcvol	432.640	ml/mol	McGowan Method
pc	742.05	kPa	Joback Method
rinpol	3559.00		NIST Webbook
tb	1150.98	K	Joback Method
tc	1431.74	K	Joback Method
tf	686.30	K	Joback Method
vc	1.696	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1519.48	J/mol×K	1150.98	Joback Method
cpg	1534.61	J/mol×K	1197.77	Joback Method
cpg	1547.43	J/mol×K	1244.57	Joback Method
cpg	1558.08	J/mol×K	1291.36	Joback Method
cpg	1566.70	J/mol×K	1338.16	Joback Method
cpg	1573.44	J/mol×K	1384.95	Joback Method
cpg	1578.43	J/mol×K	1431.74	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U377814&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