Phthalic acid, 3-fluorophenyl hexadecyl ester

Inchi: InChI=1S/C30H41FO4/c1-2-3-4-5-6-7-8-9-10-11-12-13-14-17-23-34-29(32)27-21-15-16-2
InchiKey: WAPFMLKVJPGTED-UHFFFAOYSA-N
Formula: C30H41FO4
SMILES: CCCCCCCCCCCCCCCCOC(=O)c1ccccc1C(=O)Oc1cccc(F)c1
Mol. weight [g/mol]: 484.64

Physical Properties

Property code	Value	Unit	Source
gf	-255.37	kJ/mol	Joback Method
hf	-898.12	kJ/mol	Joback Method
hfus	69.41	kJ/mol	Joback Method
hvap	105.75	kJ/mol	Joback Method
log10ws	-10.41		Crippen Method
logp	8.683		Crippen Method
mcvol	402.690	ml/mol	McGowan Method
pc	855.46	kPa	Joback Method
rinpol	3468.00		NIST Webbook
rinpol	3468.00		NIST Webbook
tb	1100.97	K	Joback Method
tc	1353.59	K	Joback Method
tf	650.65	K	Joback Method
vc	1.565	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1389.85	J/mol×K	1100.97	Joback Method
cpg	1404.73	J/mol×K	1143.07	Joback Method
cpg	1417.75	J/mol×K	1185.18	Joback Method
cpg	1429.02	J/mol×K	1227.28	Joback Method
cpg	1438.64	J/mol×K	1269.38	Joback Method
cpg	1446.72	J/mol×K	1311.48	Joback Method
cpg	1453.34	J/mol×K	1353.59	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=U356664&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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