Phthalic acid, 3-fluorobenzyl heptadecyl ester

Inchi: InChI=1S/C32H45FO4/c1-2-3-4-5-6-7-8-9-10-11-12-13-14-15-18-24-36-31(34)29-22-16-1

InchiKey: QMGWCVBQWYTFHM-UHFFFAOYSA-N

Formula: C32H45FO4

SMILES: CCCCCCCCCCCCCCCCCCOC(=O)c1ccccc1C(=O)OCc1cccc(F)c1

Mol. weight [g/mol]: 512.70

Physical Properties

Property code	Value	Unit	Source
gf	-238.53	kJ/mol	Joback Method
hf	-939.40	kJ/mol	Joback Method
hfus	74.59	kJ/mol	Joback Method
hvap	110.20	kJ/mol	Joback Method
log10ws	-11.10		Crippen Method
logp	9.211		Crippen Method
mcvol	430.870	ml/mol	McGowan Method
pc	766.91	kPa	Joback Method
rinpol	3664.00		NIST Webbook
rinpol	3664.00		NIST Webbook
tb	1146.73	K	Joback Method
tc	1420.08	K	Joback Method
tf	673.19	K	Joback Method
vc	1.677	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1514.81	J/mol×K	1146.73	Joback Method
cpg	1530.16	J/mol×K	1192.29	Joback Method
cpg	1543.39	J/mol×K	1237.85	Joback Method
cpg	1554.63	J/mol×K	1283.40	Joback Method
cpg	1564.03	J/mol×K	1328.96	Joback Method
cpg	1571.72	J/mol×K	1374.52	Joback Method
cpg	1577.84	J/mol×K	1420.08	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=U377901&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