Phthalic acid, heptadecyl 2,4,5-trifluorobenzyl ester

Inchi: InChI=1S/C32H43F3O4/c1-2-3-4-5-6-7-8-9-10-11-12-13-14-15-18-21-38-31(36)26-19-16

InchiKey: ZJJDAVQPNNSJFD-UHFFFAOYSA-N

Formula: C32H43F3O4

SMILES: CCCCCCCCCCCCCCCCCCOC(=O)c1ccccc1C(=O)OCc1cc(F)c(F)cc1F

Mol. weight [g/mol]: 548.68

Physical Properties

Property code	Value	Unit	Source
gf	-647.41	kJ/mol	Joback Method
hf	-1354.56	kJ/mol	Joback Method
hfus	79.98	kJ/mol	Joback Method
hvap	109.89	kJ/mol	Joback Method
log10ws	-11.76		Crippen Method
logp	9.489		Crippen Method
mcvol	434.410	ml/mol	McGowan Method
pc	718.37	kPa	Joback Method
rinpol	2923.00		NIST Webbook
rinpol	2923.00		NIST Webbook
tb	1155.23	K	Joback Method
tc	1444.58	K	Joback Method
tf	699.41	K	Joback Method
vc	1.714	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1524.07	J/mol×K	1155.23	Joback Method
cpg	1538.97	J/mol×K	1203.46	Joback Method
cpg	1551.36	J/mol×K	1251.68	Joback Method
cpg	1561.36	J/mol×K	1299.91	Joback Method
cpg	1569.13	J/mol×K	1348.13	Joback Method
cpg	1574.79	J/mol×K	1396.36	Joback Method
cpg	1578.50	J/mol×K	1444.58	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=U415507&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