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

Inchi: InChI=1S/C31H41F3O4/c1-2-3-4-5-6-7-8-9-10-11-12-13-14-17-20-37-30(35)25-18-15-16

InchiKey: AHTOKSRBHHBGDC-UHFFFAOYSA-N

Formula: C31H41F3O4

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

Mol. weight [g/mol]: 534.65

Physical Properties

Property code	Value	Unit	Source
gf	-655.83	kJ/mol	Joback Method
hf	-1333.92	kJ/mol	Joback Method
hfus	77.39	kJ/mol	Joback Method
hvap	107.66	kJ/mol	Joback Method
log10ws	-11.34		Crippen Method
logp	9.099		Crippen Method
mcvol	420.320	ml/mol	McGowan Method
pc	756.82	kPa	Joback Method
rinpol	2593.00		NIST Webbook
rinpol	2593.00		NIST Webbook
tb	1132.35	K	Joback Method
tc	1407.90	K	Joback Method
tf	688.14	K	Joback Method
vc	1.657	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1461.88	J/mol×K	1132.35	Joback Method
cpg	1476.54	J/mol×K	1178.27	Joback Method
cpg	1488.91	J/mol×K	1224.20	Joback Method
cpg	1499.08	J/mol×K	1270.12	Joback Method
cpg	1507.18	J/mol×K	1316.05	Joback Method
cpg	1513.33	J/mol×K	1361.97	Joback Method
cpg	1517.63	J/mol×K	1407.90	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U415506&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
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

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