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

Inchi: InChI=1S/C30H39F3O4/c1-2-3-4-5-6-7-8-9-10-11-12-13-16-19-36-29(34)24-17-14-15-18

InchiKey: QSUFBNATYQSWGC-UHFFFAOYSA-N

Formula: C30H39F3O4

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

Mol. weight [g/mol]: 520.62

Physical Properties

Property code	Value	Unit	Source
gf	-664.25	kJ/mol	Joback Method
hf	-1313.28	kJ/mol	Joback Method
hfus	74.80	kJ/mol	Joback Method
hvap	105.44	kJ/mol	Joback Method
log10ws	-10.92		Crippen Method
logp	8.709		Crippen Method
mcvol	406.230	ml/mol	McGowan Method
pc	798.43	kPa	Joback Method
rinpol	3636.00		NIST Webbook
rinpol	3636.00		NIST Webbook
tb	1109.47	K	Joback Method
tc	1372.84	K	Joback Method
tf	676.87	K	Joback Method
vc	1.601	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1399.90	J/mol×K	1109.47	Joback Method
cpg	1414.33	J/mol×K	1153.36	Joback Method
cpg	1426.65	J/mol×K	1197.26	Joback Method
cpg	1436.96	J/mol×K	1241.15	Joback Method
cpg	1445.35	J/mol×K	1285.05	Joback Method
cpg	1451.91	J/mol×K	1328.94	Joback Method
cpg	1456.73	J/mol×K	1372.84	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U415505&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