Phthalic acid, tridecyl 4-trifluoromethoxybenzyl ester

Inchi: InChI=1S/C29H37F3O5/c1-2-3-4-5-6-7-8-9-10-11-14-21-35-27(33)25-15-12-13-16-26(25

InchiKey: KLFPLAIVLZMIRW-UHFFFAOYSA-N

Formula: C29H37F3O5

SMILES: CCCCCCCCCCCCCOC(=O)c1ccccc1C(=O)OCc1ccc(OC(F)(F)F)cc1

Mol. weight [g/mol]: 522.60

Physical Properties

Property code	Value	Unit	Source
gf	-755.57	kJ/mol	Joback Method
hf	-1410.67	kJ/mol	Joback Method
hfus	66.76	kJ/mol	Joback Method
hvap	103.00	kJ/mol	Joback Method
log10ws	-10.37		Crippen Method
logp	8.410		Crippen Method
mcvol	398.010	ml/mol	McGowan Method
pc	859.48	kPa	Joback Method
rinpol	3187.00		NIST Webbook
rinpol	3187.00		NIST Webbook
tb	1095.82	K	Joback Method
tc	1348.89	K	Joback Method
tf	665.21	K	Joback Method
vc	1.552	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1366.88	J/mol×K	1095.82	Joback Method
cpg	1380.54	J/mol×K	1138.00	Joback Method
cpg	1392.39	J/mol×K	1180.18	Joback Method
cpg	1402.53	J/mol×K	1222.36	Joback Method
cpg	1411.09	J/mol×K	1264.54	Joback Method
cpg	1418.15	J/mol×K	1306.72	Joback Method
cpg	1423.84	J/mol×K	1348.89	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U377695&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