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

Inchi: InChI=1S/C29H37F3O4/c1-2-3-4-5-6-7-8-9-10-11-12-15-18-35-28(33)23-16-13-14-17-24

InchiKey: VIOQWBFQWCYOCY-UHFFFAOYSA-N

Formula: C29H37F3O4

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

Mol. weight [g/mol]: 506.60

Physical Properties

Property code	Value	Unit	Source
gf	-672.67	kJ/mol	Joback Method
hf	-1292.64	kJ/mol	Joback Method
hfus	72.21	kJ/mol	Joback Method
hvap	103.21	kJ/mol	Joback Method
log10ws	-10.50		Crippen Method
logp	8.319		Crippen Method
mcvol	392.140	ml/mol	McGowan Method
pc	843.58	kPa	Joback Method
rinpol	3488.00		NIST Webbook
rinpol	3488.00		NIST Webbook
tb	1086.59	K	Joback Method
tc	1339.29	K	Joback Method
tf	665.60	K	Joback Method
vc	1.546	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1338.15	J/mol×K	1086.59	Joback Method
cpg	1352.36	J/mol×K	1128.71	Joback Method
cpg	1364.63	J/mol×K	1170.82	Joback Method
cpg	1375.04	J/mol×K	1212.94	Joback Method
cpg	1383.66	J/mol×K	1255.06	Joback Method
cpg	1390.58	J/mol×K	1297.18	Joback Method
cpg	1395.86	J/mol×K	1339.29	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U415504&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

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