Phthalic acid, tridecyl 2-trifluoromethylbenzyl ester

Other names: Phthalic acid, tridecyl 2-trifluorobenzyl ester
Inchi: InChI=1S/C29H37F3O4/c1-2-3-4-5-6-7-8-9-10-11-16-21-35-27(33)24-18-13-14-19-25(24
InchiKey: FACKADYFSYIGSG-UHFFFAOYSA-N
Formula: C29H37F3O4
SMILES: CCCCCCCCCCCCCOC(=O)c1ccccc1C(=O)OCc1ccccc1C(F)(F)F
Mol. weight [g/mol]: 506.60

Physical Properties

Property code	Value	Unit	Source
gf	-650.57	kJ/mol	Joback Method
hf	-1278.45	kJ/mol	Joback Method
hfus	65.57	kJ/mol	Joback Method
hvap	100.59	kJ/mol	Joback Method
log10ws	-10.19		Crippen Method
logp	8.530		Crippen Method
mcvol	392.140	ml/mol	McGowan Method
pc	868.11	kPa	Joback Method
rinpol	3214.00		NIST Webbook
rinpol	3214.00		NIST Webbook
tb	1073.40	K	Joback Method
tc	1318.13	K	Joback Method
tf	642.98	K	Joback Method
vc	1.534	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1341.07	J/mol×K	1073.40	Joback Method
cpg	1355.98	J/mol×K	1114.19	Joback Method
cpg	1369.38	J/mol×K	1154.98	Joback Method
cpg	1381.38	J/mol×K	1195.76	Joback Method
cpg	1392.12	J/mol×K	1236.55	Joback Method
cpg	1401.71	J/mol×K	1277.34	Joback Method
cpg	1410.27	J/mol×K	1318.13	Joback Method

Sources

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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U377828&Units=SI

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