Phthalic acid, tetradecyl 2-trifluoromethylbenzyl ester

Other names: Phthalic acid, tetradecyl 2-trifluorobenzyl ester
Inchi: InChI=1S/C30H39F3O4/c1-2-3-4-5-6-7-8-9-10-11-12-17-22-36-28(34)25-19-14-15-20-26
InchiKey: NSDXZBPOZQECRT-UHFFFAOYSA-N
Formula: C30H39F3O4
SMILES: CCCCCCCCCCCCCCOC(=O)c1ccccc1C(=O)OCc1ccccc1C(F)(F)F
Mol. weight [g/mol]: 520.62

Physical Properties

Property code	Value	Unit	Source
gf	-642.15	kJ/mol	Joback Method
hf	-1299.09	kJ/mol	Joback Method
hfus	68.16	kJ/mol	Joback Method
hvap	102.81	kJ/mol	Joback Method
log10ws	-10.61		Crippen Method
logp	8.920		Crippen Method
mcvol	406.230	ml/mol	McGowan Method
pc	821.01	kPa	Joback Method
rinpol	3318.00		NIST Webbook
rinpol	3318.00		NIST Webbook
tb	1096.28	K	Joback Method
tc	1349.93	K	Joback Method
tf	654.25	K	Joback Method
vc	1.591	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1403.16	J/mol×K	1096.28	Joback Method
cpg	1418.45	J/mol×K	1138.56	Joback Method
cpg	1432.15	J/mol×K	1180.83	Joback Method
cpg	1444.39	J/mol×K	1223.11	Joback Method
cpg	1455.32	J/mol×K	1265.38	Joback Method
cpg	1465.07	J/mol×K	1307.66	Joback Method
cpg	1473.79	J/mol×K	1349.93	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=U377829&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