Phthalic acid, pentadecyl 2-trifluoromethylbenzyl ester

Other names: Phthalic acid, pentadecyl 2-trifluorobenzyl ester
Inchi: InChI=1S/C31H41F3O4/c1-2-3-4-5-6-7-8-9-10-11-12-13-18-23-37-29(35)26-20-15-16-21
InchiKey: IQSHXBPXGKZCNS-UHFFFAOYSA-N
Formula: C31H41F3O4
SMILES: CCCCCCCCCCCCCCCOC(=O)c1ccccc1C(=O)OCc1ccccc1C(F)(F)F
Mol. weight [g/mol]: 534.65

Physical Properties

Property code	Value	Unit	Source
gf	-633.73	kJ/mol	Joback Method
hf	-1319.73	kJ/mol	Joback Method
hfus	70.75	kJ/mol	Joback Method
hvap	105.04	kJ/mol	Joback Method
log10ws	-11.03		Crippen Method
logp	9.310		Crippen Method
mcvol	420.320	ml/mol	McGowan Method
pc	777.64	kPa	Joback Method
rinpol	3420.00		NIST Webbook
rinpol	3420.00		NIST Webbook
tb	1119.16	K	Joback Method
tc	1383.13	K	Joback Method
tf	665.52	K	Joback Method
vc	1.647	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1465.60	J/mol×K	1119.16	Joback Method
cpg	1481.33	J/mol×K	1163.16	Joback Method
cpg	1495.37	J/mol×K	1207.15	Joback Method
cpg	1507.88	J/mol×K	1251.15	Joback Method
cpg	1519.03	J/mol×K	1295.14	Joback Method
cpg	1528.98	J/mol×K	1339.14	Joback Method
cpg	1537.90	J/mol×K	1383.13	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=U377830&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