Phthalic acid, octadecyl 2-trifluorobenzyl ester

Inchi: InChI=1S/C34H47F3O4/c1-2-3-4-5-6-7-8-9-10-11-12-13-14-15-16-21-26-40-32(38)29-23
InchiKey: ACDCGMNQLUXNGR-UHFFFAOYSA-N
Formula: C34H47F3O4
SMILES: CCCCCCCCCCCCCCCCCCOC(=O)c1ccccc1C(=O)OCc1ccccc1C(F)(F)F
Mol. weight [g/mol]: 576.73

Physical Properties

Property code	Value	Unit	Source
gf	-608.47	kJ/mol	Joback Method
hf	-1381.65	kJ/mol	Joback Method
hfus	78.52	kJ/mol	Joback Method
hvap	111.72	kJ/mol	Joback Method
log10ws	-12.29		Crippen Method
logp	10.481		Crippen Method
mcvol	462.590	ml/mol	McGowan Method
pc	666.32	kPa	Joback Method
rinpol	3616.00		NIST Webbook
rinpol	3616.00		NIST Webbook
tb	1187.80	K	Joback Method
tc	1492.19	K	Joback Method
tf	699.33	K	Joback Method
vc	1.815	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1654.76	J/mol×K	1187.80	Joback Method
cpg	1672.17	J/mol×K	1238.53	Joback Method
cpg	1687.56	J/mol×K	1289.26	Joback Method
cpg	1701.20	J/mol×K	1339.99	Joback Method
cpg	1713.36	J/mol×K	1390.72	Joback Method
cpg	1724.33	J/mol×K	1441.46	Joback Method
cpg	1734.38	J/mol×K	1492.19	Joback Method

Sources

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=U377833&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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