Phthalic acid, hexadecyl 2-trifluoromethylbenzyl ester

Other names: Phthalic acid, hexadecyl 2-trifluorobenzyl ester
Inchi: InChI=1S/C32H43F3O4/c1-2-3-4-5-6-7-8-9-10-11-12-13-14-19-24-38-30(36)27-21-16-17
InchiKey: PKZIANHZQZOTMI-UHFFFAOYSA-N
Formula: C32H43F3O4
SMILES: CCCCCCCCCCCCCCCCOC(=O)c1ccccc1C(=O)OCc1ccccc1C(F)(F)F
Mol. weight [g/mol]: 548.68

Physical Properties

Property code	Value	Unit	Source
gf	-625.31	kJ/mol	Joback Method
hf	-1340.37	kJ/mol	Joback Method
hfus	73.34	kJ/mol	Joback Method
hvap	107.27	kJ/mol	Joback Method
log10ws	-11.45		Crippen Method
logp	9.701		Crippen Method
mcvol	434.410	ml/mol	McGowan Method
pc	737.62	kPa	Joback Method
rinpol	3521.00		NIST Webbook
rinpol	3521.00		NIST Webbook
tb	1142.04	K	Joback Method
tc	1417.83	K	Joback Method
tf	676.79	K	Joback Method
vc	1.702	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1528.36	J/mol×K	1142.04	Joback Method
cpg	1544.58	J/mol×K	1188.00	Joback Method
cpg	1559.01	J/mol×K	1233.97	Joback Method
cpg	1571.84	J/mol×K	1279.93	Joback Method
cpg	1583.26	J/mol×K	1325.90	Joback Method
cpg	1593.47	J/mol×K	1371.86	Joback Method
cpg	1602.66	J/mol×K	1417.83	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U377831&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
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

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