Phthalic acid, heptadecyl 2-trifluoromethylbenzyl ester

Other names: Phthalic acid, heptadecyl 2-trifluorobenzyl ester
Inchi: InChI=1S/C33H45F3O4/c1-2-3-4-5-6-7-8-9-10-11-12-13-14-15-20-25-39-31(37)28-22-17
InchiKey: AXDJHVSGGHGZHO-UHFFFAOYSA-N
Formula: C33H45F3O4
SMILES: CCCCCCCCCCCCCCCCCOC(=O)c1ccccc1C(=O)OCc1ccccc1C(F)(F)F
Mol. weight [g/mol]: 562.70

Physical Properties

Property code	Value	Unit	Source
gf	-616.89	kJ/mol	Joback Method
hf	-1361.01	kJ/mol	Joback Method
hfus	75.93	kJ/mol	Joback Method
hvap	109.49	kJ/mol	Joback Method
log10ws	-11.87		Crippen Method
logp	10.091		Crippen Method
mcvol	448.500	ml/mol	McGowan Method
pc	700.61	kPa	Joback Method
rinpol	3617.00		NIST Webbook
tb	1164.92	K	Joback Method
tc	1454.14	K	Joback Method
tf	688.06	K	Joback Method
vc	1.758	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1591.42	J/mol×K	1164.92	Joback Method
cpg	1608.20	J/mol×K	1213.12	Joback Method
cpg	1623.07	J/mol×K	1261.33	Joback Method
cpg	1636.27	J/mol×K	1309.53	Joback Method
cpg	1648.03	J/mol×K	1357.73	Joback Method
cpg	1658.57	J/mol×K	1405.94	Joback Method
cpg	1668.12	J/mol×K	1454.14	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=U377832&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

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