Trifluoroacetoxy hexadecane

Other names:	Hexadecyl trifluoroacetate
	Hexadecyl 2,2,2-trifluoroacetate
	1-Hexadecanol, trifluoroacetate
	Acetic acid, trifluoro-, hexadecyl ester
	1-Trifluoroacetoxyhexadecane
	Trifluoroacetic acid, hexadecyl ester
Inchi:	InChI=1S/C18H33F3O2/c1-2-3-4-5-6-7-8-9-10-11-12-13-14-15-16-23-17(22)18(19,20)21
InchiKey:	WAGHSYZLKZJUQC-UHFFFAOYSA-N
Formula:	C18H33F3O2
SMILES:	CCCCCCCCCCCCCCCCOC(=O)C(F)(F)F
Mol. weight [g/mol]:	338.45
CAS:	6222-03-3

Physical Properties

Property code	Value	Unit	Source
gf	-714.83	kJ/mol	Joback Method
hf	-1256.73	kJ/mol	Joback Method
hfus	46.99	kJ/mol	Joback Method
hvap	61.07	kJ/mol	Joback Method
log10ws	-6.88		Crippen Method
logp	6.573		Crippen Method
mcvol	277.230	ml/mol	McGowan Method
pc	1099.35	kPa	Joback Method
rinpol	1813.40		NIST Webbook
rinpol	1813.40		NIST Webbook
rinpol	1805.00		NIST Webbook
rinpol	1813.00		NIST Webbook
rinpol	1816.40		NIST Webbook
ripol	1929.00		NIST Webbook
tb	682.11	K	Joback Method
tc	843.48	K	Joback Method
tf	368.97	K	Joback Method
vc	1.111	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	815.26	J/mol×K	682.11	Joback Method
cpg	832.97	J/mol×K	709.00	Joback Method
cpg	849.87	J/mol×K	735.90	Joback Method
cpg	865.98	J/mol×K	762.79	Joback Method
cpg	881.33	J/mol×K	789.69	Joback Method
cpg	895.94	J/mol×K	816.58	Joback Method
cpg	909.86	J/mol×K	843.48	Joback Method

Sources

McGowan Method: http://link.springer.com/article/10.1007/BF02311772
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C6222033&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

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
ripol: Polar retention indices
tb: Normal Boiling Point Temperature
tc: Critical Temperature
tf: Normal melting (fusion) point
vc: Critical Volume