Octadecyl trifluoroacetate

Other names:	Octadecyl 2,2,2-trifluoroacetate
	1-Octadecanol, trifluoroacetate
	Trifluoroacetic acid, n-octadecyl ester
	Acetic acid, trifluoro-, octadecyl ester
	Trifluoroacetic acid, octadecyl ester
Inchi:	InChI=1S/C20H37F3O2/c1-2-3-4-5-6-7-8-9-10-11-12-13-14-15-16-17-18-25-19(24)20(21
InchiKey:	YZVKTRPQHJKFOD-UHFFFAOYSA-N
Formula:	C20H37F3O2
SMILES:	CCCCCCCCCCCCCCCCCCOC(=O)C(F)(F)F
Mol. weight [g/mol]:	366.50
CAS:	79392-43-1

Physical Properties

Property code	Value	Unit	Source
gf	-697.99	kJ/mol	Joback Method
hf	-1298.01	kJ/mol	Joback Method
hfus	52.17	kJ/mol	Joback Method
hvap	65.52	kJ/mol	Joback Method
log10ws	-7.72		Crippen Method
logp	7.353		Crippen Method
mcvol	305.410	ml/mol	McGowan Method
pc	971.70	kPa	Joback Method
rinpol	2006.30		NIST Webbook
rinpol	2006.30		NIST Webbook
rinpol	2008.00		NIST Webbook
rinpol	2001.00		NIST Webbook
rinpol	2001.00		NIST Webbook
ripol	2121.00		NIST Webbook
tb	727.87	K	Joback Method
tc	894.11	K	Joback Method
tf	391.51	K	Joback Method
vc	1.222	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	932.92	J/mol×K	727.87	Joback Method
cpg	951.62	J/mol×K	755.58	Joback Method
cpg	969.43	J/mol×K	783.28	Joback Method
cpg	986.37	J/mol×K	810.99	Joback Method
cpg	1002.48	J/mol×K	838.70	Joback Method
cpg	1017.78	J/mol×K	866.40	Joback Method
cpg	1032.32	J/mol×K	894.11	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=C79392431&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
ripol:	Polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume