Heptadecyl trifluoroacetate

Other names: Heptadecyl 2,2,2-trifluoroacetate
1-Heptadecanol, trifluoroacetate
Trifluoroacetic acid, n-heptadecyl ester
Inchi: InChI=1S/C19H35F3O2/c1-2-3-4-5-6-7-8-9-10-11-12-13-14-15-16-17-24-18(23)19(20,21
InchiKey: CDOYOXVOYRQINU-UHFFFAOYSA-N
Formula: C19H35F3O2
SMILES: CCCCCCCCCCCCCCCCCOC(=O)C(F)(F)F
Mol. weight [g/mol]: 352.48

Physical Properties

Property code	Value	Unit	Source
gf	-706.41	kJ/mol	Joback Method
hf	-1277.37	kJ/mol	Joback Method
hfus	49.58	kJ/mol	Joback Method
hvap	63.30	kJ/mol	Joback Method
log10ws	-7.30		Crippen Method
logp	6.963		Crippen Method
mcvol	291.320	ml/mol	McGowan Method
pc	1032.57	kPa	Joback Method
rinpol	1907.00		NIST Webbook
rinpol	1910.20		NIST Webbook
tb	704.99	K	Joback Method
tc	868.50	K	Joback Method
tf	380.24	K	Joback Method
vc	1.167	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	873.58	J/mol×K	704.99	Joback Method
cpg	891.77	J/mol×K	732.24	Joback Method
cpg	909.12	J/mol×K	759.49	Joback Method
cpg	925.64	J/mol×K	786.74	Joback Method
cpg	941.36	J/mol×K	813.99	Joback Method

cpg	956.32	J/mol×K	841.24	Joback Method
cpg	970.55	J/mol×K	868.50	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=U351870&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