Trifluoroacetic acid, pentadecyl ester

Other names: Pentadecyl trifluoroacetate
Inchi: InChI=1S/C17H31F3O2/c1-2-3-4-5-6-7-8-9-10-11-12-13-14-15-22-16(21)17(18,19)20/h2-
InchiKey: WXLYYNRKQJZZGJ-UHFFFAOYSA-N
Formula: C17H31F3O2
SMILES: CCCCCCCCCCCCCCCOC(=O)C(F)(F)F
Mol. weight [g/mol]: 324.42
CAS: 959010-23-2

Physical Properties

Property code	Value	Unit	Source
gf	-723.25	kJ/mol	Joback Method
hf	-1236.09	kJ/mol	Joback Method
hfus	44.40	kJ/mol	Joback Method
hvap	58.84	kJ/mol	Joback Method
log10ws	-6.46		Crippen Method
logp	6.183		Crippen Method
mcvol	263.140	ml/mol	McGowan Method
pc	1172.83	kPa	Joback Method
rinpol	1717.00		NIST Webbook
rinpol	1726.60		NIST Webbook
rinpol	1717.00		NIST Webbook
rinpol	1726.60		NIST Webbook
tb	659.23	K	Joback Method
tc	819.00	K	Joback Method
tf	357.70	K	Joback Method
vc	1.054	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	758.05	J/mol×K	659.23	Joback Method
cpg	775.28	J/mol×K	685.86	Joback Method
cpg	791.74	J/mol×K	712.49	Joback Method
cpg	807.44	J/mol×K	739.11	Joback Method

cpg	822.41	J/mol×K	765.74	Joback Method
cpg	836.69	J/mol×K	792.37	Joback Method
cpg	850.28	J/mol×K	819.00	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C959010232&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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume