Ethanethioic acid S-tert-butyl ester

Other names:	CH3C(O)SC(CH3)3
	S-tert-Butyl thioacetate
	t-Butyl thiolacetate
Inchi:	InChI=1S/C6H12OS/c1-5(7)8-6(2,3)4/h1-4H3
InchiKey:	PJFHXBBYLAVSLJ-UHFFFAOYSA-N
Formula:	C6H12OS
SMILES:	CC(=O)SC(C)(C)C
Mol. weight [g/mol]:	132.22
CAS:	999-90-6

Physical Properties

Property code	Value	Unit	Source
gf	-93.32	kJ/mol	Joback Method
hf	-246.63	kJ/mol	Joback Method
hfus	9.61	kJ/mol	Joback Method
hvap	42.90 ± 0.20	kJ/mol	NIST Webbook
hvap	42.90 ± 0.20	kJ/mol	NIST Webbook
log10ws	-2.10		Crippen Method
logp	2.065		Crippen Method
mcvol	113.320	ml/mol	McGowan Method
pc	3480.65	kPa	Joback Method
rinpol	834.00		NIST Webbook
rinpol	834.00		NIST Webbook
tb	405.00 ± 4.00	K	NIST Webbook
tc	670.46	K	Joback Method
tf	244.13	K	Joback Method
vc	0.420	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	226.34	J/mol×K	456.10	Joback Method
cpg	238.36	J/mol×K	491.83	Joback Method
cpg	249.68	J/mol×K	527.55	Joback Method

cpg	260.33	J/mol×K	563.28	Joback Method
cpg	270.33	J/mol×K	599.01	Joback Method
cpg	279.71	J/mol×K	634.74	Joback Method
cpg	288.49	J/mol×K	670.46	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=C999906&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