ETHANETHIOIC ACID, S-(1,1-DIMETHYLETHYL) 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]: 132.23

Physical Properties

Property code	Value	Unit	Source
hf	-290.45	kJ/mol	Cheméo Relay (1.0)
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
ie	9.08	eV	Cheméo Relay (1.0)
log10ws	-1.53		Cheméo Relay (1.0)
logp	2.065		Crippen Method
mcvol	113.320	ml/mol	McGowan Method
rinpol	834.00		NIST Webbook
rinpol	834.00		NIST Webbook
tb	405.00 ± 4.00	K	NIST Webbook
tc	591.37	K	Cheméo Relay (1.0)
tf	255.15	K	Cheméo Relay (1.0)

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
Cheméo Relay (1.0):	
Cheméo Relay (1.0, beta):	
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C999906&Units=SI
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

Legend

cpg:	Ideal gas heat capacity
hf:	Enthalpy of formation at standard conditions
hfus:	Enthalpy of fusion at standard conditions
hvap:	Enthalpy of vaporization at standard conditions
ie:	Ionization energy
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point