sec-Butyl t-butyl sulfide

Other names: 3,5,5-trimethyl-4-thiahexane
Inchi: InChI=1S/C8H18S/c1-6-7(2)9-8(3,4)5/h7H,6H2,1-5H3
InchiKey: GARAYLGABNDHRH-UHFFFAOYSA-N
Formula: C8H18S
SMILES: CCC(C)SC(C)(C)C
Mol. weight [g/mol]: 146.29

Physical Properties

Property code	Value	Unit	Source
gf	50.00	kJ/mol	Joback Method
hf	-180.61	kJ/mol	Joback Method
hfus	9.67	kJ/mol	Joback Method
hvap	38.54	kJ/mol	Joback Method
log10ws	-3.28		Crippen Method
logp	3.317		Crippen Method
mcvol	139.930	ml/mol	McGowan Method
pc	2651.56	kPa	Joback Method
rinpol	934.00		NIST Webbook
rinpol	934.00		NIST Webbook
rinpol	952.00		NIST Webbook
rinpol	934.00		NIST Webbook
rinpol	934.00		NIST Webbook
tb	447.55	K	Joback Method
tc	649.97	K	Joback Method
tf	201.74	K	Joback Method
vc	0.520	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	289.43	J/mol×K	447.55	Joback Method
cpg	305.13	J/mol×K	481.29	Joback Method
cpg	320.01	J/mol×K	515.02	Joback Method
cpg	334.09	J/mol×K	548.76	Joback Method

cpg	347.41	J/mol×K	582.50	Joback Method
cpg	359.99	J/mol×K	616.23	Joback Method
cpg	371.87	J/mol×K	649.97	Joback Method

Sources

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=U343637&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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