Propane, 2-methyl-2-[(1-methylethyl)thio]-

Other names: tert-Butyl isopropyl sulfide
2,4,4-Trimethyl-3-thiapentane
Sulfide, tert-butyl isopropyl
Isopropyl tert-butyl sulfide
Inchi: InChI=1S/C7H16S/c1-6(2)8-7(3,4)5/h6H,1-5H3
InchiKey: OBGJHUWOEJFPJS-UHFFFAOYSA-N
Formula: C7H16S
SMILES: CC(C)SC(C)(C)C
Mol. weight [g/mol]: 132.27
CAS: 44657-76-3

Physical Properties

Property code	Value	Unit	Source
gf	41.58	kJ/mol	Joback Method
hf	-159.97	kJ/mol	Joback Method
hfus	7.08	kJ/mol	Joback Method
hvap	36.31	kJ/mol	Joback Method
log10ws	-2.86		Crippen Method
logp	2.926		Crippen Method
mcvol	125.840	ml/mol	McGowan Method
pc	2934.52	kPa	Joback Method
rinpol	835.00		NIST Webbook
rinpol	835.00		NIST Webbook
rinpol	835.00		NIST Webbook
rinpol	835.00		NIST Webbook
tb	424.67	K	Joback Method
tc	629.44	K	Joback Method
tf	190.47	K	Joback Method
vc	0.465	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	247.76	J/mol×K	424.67	Joback Method

cpg	262.38	J/mol×K	458.80	Joback Method
cpg	276.23	J/mol×K	492.93	Joback Method
cpg	289.33	J/mol×K	527.06	Joback Method
cpg	301.71	J/mol×K	561.18	Joback Method
cpg	313.40	J/mol×K	595.31	Joback Method
cpg	324.42	J/mol×K	629.44	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C44657763&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
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

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