Propane, 2-(ethylthio)-2-methyl-

Other names:	1-(tert-Butylthio)ethane
	2,2-Dimethyl-3-thiapentane
	2-(Ethylthio)-2-methyl-propane
	Ethyl tert-butyl sulfide
	Sulfide, tert-butyl ethyl
	tert-Butyl ethyl sulfide
	tert-Butyl ethyl sulphide
Inchi:	InChI=1S/C6H14S/c1-5-7-6(2,3)4/h5H2,1-4H3
InchiKey:	GZJUDUMQICJSFJ-UHFFFAOYSA-N
Formula:	C6H14S
SMILES:	CCSC(C)(C)C
Mol. weight [g/mol]:	118.24
CAS:	14290-92-7

Physical Properties

Property code	Value	Unit	Source
chl	-4776.90 ± 2.10	kJ/mol	NIST Webbook
gf	35.60	kJ/mol	Joback Method
hf	-148.00 ± 3.00	kJ/mol	NIST Webbook
hfl	-187.00 ± 2.00	kJ/mol	NIST Webbook
hfus	8.01	kJ/mol	Joback Method
hvap	39.00	kJ/mol	NIST Webbook
hvap	39.00 ± 1.00	kJ/mol	NIST Webbook
hvap	39.30	kJ/mol	NIST Webbook
log10ws	-2.33		Crippen Method
logp	2.538		Crippen Method
mcvol	111.750	ml/mol	McGowan Method
pc	3235.66	kPa	Joback Method
rinpol	792.00		NIST Webbook
rinpol	792.00		NIST Webbook
rinpol	782.00		NIST Webbook
rinpol	792.00		NIST Webbook
rinpol	792.00		NIST Webbook
rinpol	792.00		NIST Webbook
tb	393.56 ± 0.30	K	NIST Webbook
tb	390.30 ± 2.00	K	NIST Webbook
tb	393.56 ± 0.30	K	NIST Webbook

tb	393.30 ± 0.40	K	NIST Webbook
tb	393.60 ± 0.30	K	NIST Webbook
tc	604.13	K	Joback Method
tf	184.20 ± 0.20	K	NIST Webbook
tf	187.20 ± 0.20	K	NIST Webbook
vc	0.414	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	256.20	J/mol×K	536.83	Joback Method
cpg	266.61	J/mol×K	570.48	Joback Method
cpg	208.29	J/mol×K	402.23	Joback Method
cpg	221.25	J/mol×K	435.88	Joback Method
cpg	233.54	J/mol×K	469.53	Joback Method
cpg	245.18	J/mol×K	503.18	Joback Method
cpg	276.44	J/mol×K	604.13	Joback Method
hvapt	39.20	kJ/mol	356.50	NIST Webbook
hvapt	37.10	kJ/mol	366.00	NIST Webbook

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.50819e+01
Coeff. B	-3.55490e+03
Coeff. C	-5.05600e+01
Temperature range (K), min.	290.85
Temperature range (K), max.	414.40

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C14290927&Units=SI

The Yaws Handbook of Vapor Pressure: https://www.sciencedirect.com/book/9780128029992/the-yaws-handbook-of-vapor-pressure

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
KDB:	https://www.cheric.org/files/research/kdb/mol/mol1838.mol
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

Legend

chl:	Standard liquid enthalpy of combustion
cpg:	Ideal gas heat capacity
gf:	Standard Gibbs free energy of formation
hf:	Enthalpy of formation at standard conditions
hfl:	Liquid phase enthalpy of formation at standard conditions
hfus:	Enthalpy of fusion at standard conditions
hvap:	Enthalpy of vaporization at standard conditions
hvapt:	Enthalpy of vaporization at a given temperature
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
pc:	Critical Pressure
pvap:	Vapor pressure
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume