Disulfide, 1,1-dimethylethyl ethyl

Other names:	2,2-Dimethyl-3,4-dithiahexane
	2-Methyl-2-propyl ethyl disulfide
	Disulfide, tert-butyl ethyl
	Ethyl t-butyl disulfide
	Ethyl tert-butyl disulfide
	tert-Butyl Ethyl disulfide
Inchi:	InChI=1S/C6H14S2/c1-5-7-8-6(2,3)4/h5H2,1-4H3
InchiKey:	CLMXSBZIYJITQU-UHFFFAOYSA-N
Formula:	C6H14S2
SMILES:	CCSSC(C)(C)C
Mol. weight [g/mol]:	150.31
CAS:	4151-69-3

Physical Properties

Property code	Value	Unit	Source
gf	68.72	kJ/mol	Joback Method
hf	-92.18	kJ/mol	Joback Method
hfus	12.14	kJ/mol	Joback Method
hvap	41.29	kJ/mol	Joback Method
ie	8.20 ± 0.80	eV	NIST Webbook
log10ws	-3.20		Crippen Method
logp	3.186		Crippen Method
mcvol	128.100	ml/mol	McGowan Method
pc	3299.15	kPa	Joback Method
rinpol	1023.00		NIST Webbook
rinpol	1023.00		NIST Webbook
rinpol	1023.00		NIST Webbook
ripol	1299.00		NIST Webbook
tb	448.00 ± 1.50	K	NIST Webbook
tc	697.89	K	Joback Method
tf	206.40 ± 0.20	K	NIST Webbook
vc	0.469	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	257.06	J/mol×K	471.01	Joback Method
cpg	270.59	J/mol×K	508.82	Joback Method
cpg	283.33	J/mol×K	546.64	Joback Method
cpg	295.30	J/mol×K	584.45	Joback Method
cpg	306.53	J/mol×K	622.27	Joback Method
cpg	317.05	J/mol×K	660.08	Joback Method
cpg	326.87	J/mol×K	697.89	Joback Method
hvapt	43.40	kJ/mol	417.00	NIST Webbook

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.40333e+01
Coeff. B	-3.59032e+03
Coeff. C	-6.66580e+01
Temperature range (K), min.	327.85
Temperature range (K), max.	478.31

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C4151693&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

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
hvapt:	Enthalpy of vaporization at a given temperature
ie:	Ionization energy
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
ripol:	Polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume