Di-tert-butyl disulfide

Other names:	(tert-C4H9S)2
	2,2,5,5-Tetramethyl-3,4-dithiahexane
	2-(tert-Butyldisulfanyl)-2-methylpropane
	Bis(1,1-dimethylethyl) disulfide
	Bis(1,1-dimethylethyl) disulphide
	Di-tert-butyl disulphide
	Disulfide, bis(1,1-dimethylethyl)
	t-Butyl disulfide
	tert-Butyl disulfide
Inchi:	InChI=1S/C8H18S2/c1-7(2,3)9-10-8(4,5)6/h1-6H3
InchiKey:	BKCNDTDWDGQHSD-UHFFFAOYSA-N
Formula:	C8H18S2
SMILES:	CC(C)(C)SSC(C)(C)C
Mol. weight [g/mol]:	178.36
CAS:	110-06-5

Physical Properties

Property code	Value	Unit	Source
chl	-6674.10 ± 1.60	kJ/mol	NIST Webbook
chl	-6670.00 ± 1.30	kJ/mol	NIST Webbook
gf	88.40	kJ/mol	Joback Method
hf	-202.00 ± 2.30	kJ/mol	NIST Webbook
hf	-199.80 ± 2.30	kJ/mol	NIST Webbook
hf	-200.00	kJ/mol	NIST Webbook
hfl	-251.00 ± 1.80	kJ/mol	NIST Webbook
hfl	-253.00 ± 1.50	kJ/mol	NIST Webbook
hfus	9.91	kJ/mol	Joback Method
hvap	53.80	kJ/mol	NIST Webbook
hvap	52.50 ± 0.20	kJ/mol	NIST Webbook
hvap	52.50	kJ/mol	NIST Webbook
hvap	49.00	kJ/mol	NIST Webbook
hvap	53.00 ± 2.00	kJ/mol	NIST Webbook
hvap	54.27	kJ/mol	NIST Webbook
hvap	53.00 ± 2.00	kJ/mol	NIST Webbook
hvap	53.20	kJ/mol	NIST Webbook
ie	8.15	eV	NIST Webbook
ie	8.17	eV	NIST Webbook

ie	8.20	eV	NIST Webbook
ie	8.17	eV	NIST Webbook
log10ws	-4.15		Crippen Method
logp	3.965		Crippen Method
mcvol	156.280	ml/mol	McGowan Method
pc	2729.71	kPa	Joback Method
rinpol	1122.00		NIST Webbook
rinpol	1122.00		NIST Webbook
ripol	1331.00		NIST Webbook
ripol	1364.00		NIST Webbook
ripol	1323.00		NIST Webbook
ripol	1323.00		NIST Webbook
tb	473.70	K	NIST Webbook
tc	747.84	K	Joback Method
tf	253.56	K	Joback Method
vc	0.570	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	347.09	J/mol×K	513.54	Joback Method
cpg	363.97	J/mol×K	552.59	Joback Method
cpg	379.66	J/mol×K	591.64	Joback Method
cpg	394.24	J/mol×K	630.69	Joback Method
cpg	407.75	J/mol×K	669.74	Joback Method
cpg	420.26	J/mol×K	708.79	Joback Method
cpg	431.83	J/mol×K	747.84	Joback Method

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	361.20	K	2.80	NIST Webbook

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.32257e+01
Coeff. B	-3.68705e+03
Coeff. C	-7.54240e+01
Temperature range (K), min.	360.40
Temperature range (K), max.	541.30

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C110065&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

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
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
tbrp:	Boiling point at reduced pressure
tc:	Critical Temperature

tf: Normal melting (fusion) point

vc: Critical Volume