Di-tert-butyl sulfide

Other names:	(tert-C4H9)2S
	2,2'-Thiobis(2-methyl-propane)
	2,2,4,4-Tetramethyl-3-thiapentane
	2-(tert-Butylsulfanyl)-2-methylpropane
	Di-tert-butyl sulphide
	NSC 4549
	Propane, 2,2'-thiobis[2-methyl-
	t-Butyl sulfide
	tert-Butyl sulfide
Inchi:	InChI=1S/C8H18S/c1-7(2,3)9-8(4,5)6/h1-6H3
InchiKey:	LNMBCRKRCIMQLW-UHFFFAOYSA-N
Formula:	C8H18S
SMILES:	CC(C)(C)SC(C)(C)C
Mol. weight [g/mol]:	146.29
CAS:	107-47-1

Physical Properties

Property code	Value	Unit	Source
affp	893.80	kJ/mol	NIST Webbook
basg	864.00	kJ/mol	NIST Webbook
chl	-6090.36 ± 0.92	kJ/mol	NIST Webbook
chl	-6090.15 ± 0.75	kJ/mol	NIST Webbook
gf	55.28	kJ/mol	Joback Method
hf	-188.50 ± 1.10	kJ/mol	NIST Webbook
hf	-187.00 ± 2.70	kJ/mol	NIST Webbook
hfl	-232.30 ± 1.10	kJ/mol	NIST Webbook
hfl	-232.70 ± 0.96	kJ/mol	NIST Webbook
hfus	5.78	kJ/mol	Joback Method
hvap	45.70	kJ/mol	NIST Webbook
hvap	45.61 ± 0.92	kJ/mol	NIST Webbook
hvap	43.80	kJ/mol	NIST Webbook
hvap	43.80 ± 0.20	kJ/mol	NIST Webbook
hvap	43.79	kJ/mol	NIST Webbook
ie	8.07	eV	NIST Webbook
ie	8.07	eV	NIST Webbook
ie	8.18 ± 0.05	eV	NIST Webbook
ie	8.20 ± 0.10	eV	NIST Webbook

log10ws	-3.28		Crippen Method
logp	3.317		Crippen Method
mcvol	139.930	ml/mol	McGowan Method
pc	2681.86	kPa	Joback Method
rinpol	918.00		NIST Webbook
rinpol	905.00		NIST Webbook
rinpol	918.00		NIST Webbook
rinpol	918.00		NIST Webbook
rinpol	913.00		NIST Webbook
rinpol	927.00		NIST Webbook
rinpol	920.00		NIST Webbook
tb	422.20	K	NIST Webbook
tb	422.20	K	NIST Webbook
tc	656.01	K	Joback Method
tf	219.16	K	Joback Method
vc	0.515	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	291.66	J/mol×K	444.76	Joback Method
cpg	308.46	J/mol×K	479.97	Joback Method
cpg	324.21	J/mol×K	515.18	Joback Method
cpg	338.96	J/mol×K	550.39	Joback Method
cpg	352.75	J/mol×K	585.59	Joback Method
cpg	365.64	J/mol×K	620.80	Joback Method
cpg	377.69	J/mol×K	656.01	Joback Method
hvapt	33.26	kJ/mol	422.20	NIST Webbook

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.48165e+01
Coeff. B	-3.70872e+03
Coeff. C	-5.85350e+01
Temperature range (K), min.	313.80

Temperature range (K), max.	448.72

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C107471&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

Legend

affp:	Proton affinity
basg:	Gas basicity
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
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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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