

Disulfide, (1-methylethyl) (1,1-dimethylethyl)

Other names:	2,5,5-Trimethyl-3,4-dithiahexane
Inchi:	InChI=1S/C7H16S2/c1-6(2)8-9-7(3,4)5/h6H,1-5H3
InchiKey:	ZWAYVJUPUDGBIH-UHFFFAOYSA-N
Formula:	C7H16S2
SMILES:	CC(C)SSC(C)(C)C
Mol. weight [g/mol]:	164.33
CAS:	43022-60-2

Physical Properties

Property code	Value	Unit	Source
gf	74.70	kJ/mol	Joback Method
hf	-167.00	kJ/mol	NIST Webbook
hfus	11.21	kJ/mol	Joback Method
hvap	43.13	kJ/mol	Joback Method
ie	8.10 ± 0.80	eV	NIST Webbook
log10ws	-3.73		Crippen Method
logp	3.575		Crippen Method
mcvol	142.190	ml/mol	McGowan Method
pc	2989.32	kPa	Joback Method
rinpol	1060.00		NIST Webbook
rinpol	1060.00		NIST Webbook
rinpol	1060.00		NIST Webbook
ripol	1308.00		NIST Webbook
tb	493.45	K	Joback Method
tc	721.94	K	Joback Method
tf	224.87	K	Joback Method
vc	0.518	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	299.74	J/molxK	493.45	Joback Method
cpg	314.82	J/molxK	531.53	Joback Method
cpg	329.00	J/molxK	569.61	Joback Method

cpg	342.32	J/mol×K	607.69	Joback Method
cpg	354.78	J/mol×K	645.77	Joback Method
cpg	366.44	J/mol×K	683.86	Joback Method
cpg	377.31	J/mol×K	721.94	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C43022602&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Joback Method:	https://en.wikipedia.org/wiki/Joback_method

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
ie:	Ionization energy
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
pc:	Critical Pressure
rinpola:	Non-polar retention indices
ripola:	Polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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