

1,3-Dithiolane, 2,2-dimethyl-

Other names:	2,2-Dimethyl-1,3-dithiolane
Inchi:	InChI=1S/C5H10S2/c1-5(2)6-3-4-7-5/h3-4H2,1-2H3
InchiKey:	HEDYXMHGMMWNBO-UHFFFAOYSA-N
Formula:	C5H10S2
SMILES:	CC1(C)SCCS1
Mol. weight [g/mol]:	134.26
CAS:	6008-78-2

Physical Properties

Property code	Value	Unit	Source
gf	102.00	kJ/mol	Joback Method
hf	19.71	kJ/mol	Joback Method
hfus	3.66	kJ/mol	Joback Method
hvap	37.45	kJ/mol	Joback Method
log10ws	-2.18		Crippen Method
logp	2.202		Crippen Method
mcvol	103.150	ml/mol	McGowan Method
pc	4534.68	kPa	Joback Method
rinpol	1032.00		NIST Webbook
rinpol	1032.00		NIST Webbook
tb	424.98	K	Joback Method
tc	669.18	K	Joback Method
tf	347.81	K	Joback Method
vc	0.346	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	187.46	J/mol×K	424.98	Joback Method
cpg	200.86	J/mol×K	465.68	Joback Method
cpg	212.99	J/mol×K	506.38	Joback Method
cpg	224.02	J/mol×K	547.08	Joback Method
cpg	234.11	J/mol×K	587.78	Joback Method
cpg	243.43	J/mol×K	628.48	Joback Method

Sources

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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C6008782&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
pc:	Critical 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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