

2,4-Dimethyl-1,3-dithiolane

Other names:	2,4-Dimethyl-1,3-dithiolan
Inchi:	InChI=1S/C5H10S2/c1-4-3-6-5(2)7-4/h4-5H,3H2,1-2H3
InchiKey:	FSCICYWMDXUMTJ-UHFFFAOYSA-N
Formula:	C5H10S2
SMILES:	CC1CSC(C)S1
Mol. weight [g/mol]:	134.26

Physical Properties

Property code	Value	Unit	Source
gf	99.78	kJ/mol	Joback Method
hf	-15.87	kJ/mol	Joback Method
hfus	11.03	kJ/mol	Joback Method
hvap	38.30	kJ/mol	Joback Method
log10ws	-2.30		Crippen Method
logp	2.201		Crippen Method
mcvol	103.150	ml/mol	McGowan Method
pc	4093.38	kPa	Joback Method
rinpol	1044.00		NIST Webbook
rinpol	1012.00		NIST Webbook
rinpol	1050.00		NIST Webbook
rinpol	1032.00		NIST Webbook
rinpol	1032.00		NIST Webbook
rinpol	1032.00		NIST Webbook
rinpol	1060.00		NIST Webbook
rinpol	1032.00		NIST Webbook
rinpol	1078.00		NIST Webbook
rinpol	1060.00		NIST Webbook
rinpol	1060.00		NIST Webbook
rinpol	1012.00		NIST Webbook
tb	420.07	K	Joback Method
tc	652.62	K	Joback Method
tf	319.67	K	Joback Method
vc	0.347	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	187.50	J/mol×K	420.07	Joback Method
cpg	200.81	J/mol×K	458.83	Joback Method
cpg	213.36	J/mol×K	497.59	Joback Method
cpg	225.19	J/mol×K	536.35	Joback Method
cpg	236.31	J/mol×K	575.10	Joback Method
cpg	246.76	J/mol×K	613.86	Joback Method
cpg	256.56	J/mol×K	652.62	Joback Method

Sources

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
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R78773&Units=SI

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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