

cis-2-(mercaptomethyl)-4-methyl-1,3-dioxolane

Inchi:	InChI=1S/C5H10O2S/c1-4-2-6-5(3-8)7-4/h4-5,8H,2-3H2,1H3/t4-,5+/m1/s1
InchiKey:	IZIJAPPJBKUSNQ-UHNVWZDZSA-N
Formula:	C5H10O2S
SMILES:	CC1COC(CS)O1
Mol. weight [g/mol]:	134.20

Physical Properties

Property code	Value	Unit	Source
gf	-122.79	kJ/mol	Joback Method
hf	-331.91	kJ/mol	Joback Method
hfus	23.71	kJ/mol	Joback Method
hvap	42.43	kJ/mol	Joback Method
log10ws	-0.78		Crippen Method
logp	0.678		Crippen Method
mcvol	98.540	ml/mol	McGowan Method
pc	4414.96	kPa	Joback Method
rinpol	959.00		NIST Webbook
rinpol	959.00		NIST Webbook
ripol	1454.00		NIST Webbook
tb	441.17	K	Joback Method
tc	665.59	K	Joback Method
tf	242.37	K	Joback Method
vc	0.351	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	203.21	J/molxK	441.17	Joback Method
cpg	216.16	J/molxK	478.57	Joback Method
cpg	228.42	J/molxK	515.98	Joback Method
cpg	240.00	J/molxK	553.38	Joback Method
cpg	250.93	J/molxK	590.78	Joback Method
cpg	261.21	J/molxK	628.18	Joback Method
cpg	270.86	J/molxK	665.59	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=R169294&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
rinpolar:	Non-polar retention indices
ripolar:	Polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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