4,5-dimethyl-1,3-dithiolane

Other names: 4,5-Dimethyl-1,3-dithiolan
Inchi: InChI=1S/C5H10S2/c1-4-5(2)7-3-6-4/h4-5H,3H2,1-2H3
InchiKey: VDKQRNZRLREXBM-UHFFFAOYSA-N
Formula: C5H10S2
SMILES: CC1SCSC1C
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	1090.00		NIST Webbook
rinpol	1090.00		NIST Webbook
rinpol	1090.00		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

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=R125912&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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