2,2,4-Trimethyl-1,3-dithiolane

Inchi: InChI=1S/C6H12S2/c1-5-4-7-6(2,3)8-5/h5H,4H2,1-3H3
InchiKey: CRVLTUAGMFKJEA-UHFFFAOYSA-N
Formula: C6H12S2
SMILES: CC1CSC(C)(C)S1
Mol. weight [g/mol]: 148.29
CAS: 5862-53-3

Physical Properties

Property code	Value	Unit	Source
gf	102.71	kJ/mol	Joback Method
hf	-21.27	kJ/mol	Joback Method
hfus	7.32	kJ/mol	Joback Method
hvap	39.37	kJ/mol	Joback Method
log10ws	-2.72		Crippen Method
logp	2.591		Crippen Method
mcvol	117.240	ml/mol	McGowan Method
pc	3838.78	kPa	Joback Method
rinpol	1063.00		NIST Webbook
tb	443.19	K	Joback Method
tc	683.19	K	Joback Method
tf	354.84	K	Joback Method
vc	0.402	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	227.79	J/mol×K	443.19	Joback Method
cpg	242.75	J/mol×K	483.19	Joback Method
cpg	256.49	J/mol×K	523.19	Joback Method
cpg	269.14	J/mol×K	563.19	Joback Method
cpg	280.87	J/mol×K	603.19	Joback Method
cpg	291.81	J/mol×K	643.19	Joback Method
cpg	302.13	J/mol×K	683.19	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=C5862533&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