1,3-Dithiolo[4,5-b]furan, tetrahydro-3a-methyl-

Other names: 1-Methylbicyclo[3.3.0]-2,4-dithia-8-oxaoctane
Inchi: InChI=1S/C6H10OS2/c1-6-5(2-3-7-6)8-4-9-6/h5H,2-4H2,1H3
InchiKey: NMEFNVFVAKLNKO-UHFFFAOYSA-N
Formula: C6H10OS2
SMILES: CC12OCCC1SCS2
Mol. weight [g/mol]: 162.27
CAS: 67411-25-0

Physical Properties

Property code	Value	Unit	Source
gf	85.05	kJ/mol	Joback Method
hf	-60.13	kJ/mol	Joback Method
hfus	12.36	kJ/mol	Joback Method
hvap	44.10	kJ/mol	Joback Method
log10ws	-2.19		Crippen Method
logp	1.929		Crippen Method
mcvol	112.250	ml/mol	McGowan Method
pc	4691.31	kPa	Joback Method
rinpol	1245.00		NIST Webbook
tb	481.55	K	Joback Method
tc	740.83	K	Joback Method
tf	403.59	K	Joback Method
vc	0.381	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	239.85	J/mol×K	481.55	Joback Method
cpg	254.75	J/mol×K	524.76	Joback Method
cpg	268.11	J/mol×K	567.98	Joback Method
cpg	280.19	J/mol×K	611.19	Joback Method
cpg	291.23	J/mol×K	654.40	Joback Method
cpg	301.47	J/mol×K	697.62	Joback Method
cpg	311.16	J/mol×K	740.83	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C67411250&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Joback Method:	https://en.wikipedia.org/wiki/Joback_method

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