3-Methyl-1,2-dithiolane

Inchi: InChI=1S/C4H8S2/c1-4-2-3-5-6-4/h4H,2-3H2,1H3
InchiKey: YGRXDUYBUNBNHK-UHFFFAOYSA-N
Formula: C4H8S2
SMILES: CC1CCSS1
Mol. weight [g/mol]: 120.24

Physical Properties

Property code	Value	Unit	Source
gf	99.07	kJ/mol	Joback Method
hf	25.11	kJ/mol	Joback Method
hfus	7.36	kJ/mol	Joback Method
hvap	36.38	kJ/mol	Joback Method
log10ws	-2.26		Crippen Method
logp	2.160		Crippen Method
mcvol	89.060	ml/mol	McGowan Method
pc	4862.97	kPa	Joback Method
rinpol	1067.00		NIST Webbook
rinpol	1067.00		NIST Webbook
tb	401.86	K	Joback Method
tc	638.04	K	Joback Method
tf	312.64	K	Joback Method
vc	0.292	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	149.32	J/mol×K	401.86	Joback Method
cpg	160.81	J/mol×K	441.22	Joback Method
cpg	171.57	J/mol×K	480.59	Joback Method
cpg	181.64	J/mol×K	519.95	Joback Method
cpg	191.04	J/mol×K	559.31	Joback Method
cpg	199.83	J/mol×K	598.68	Joback Method
cpg	208.02	J/mol×K	638.04	Joback Method

Sources

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
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R156644&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