3-methyl-1,2-dithiolan-4-one

Other names: 1,2-Dithiolan-4-one, 3-methyl
Inchi: InChI=1S/C4H6OS2/c1-3-4(5)2-6-7-3/h3H,2H2,1H3
InchiKey: ARWPSTDFVNPXSC-UHFFFAOYSA-N
Formula: C4H6OS2
SMILES: CC1SSCC1=O
Mol. weight [g/mol]: 134.22

Physical Properties

Property code	Value	Unit	Source
gf	-23.52	kJ/mol	Joback Method
hf	-112.59	kJ/mol	Joback Method
hfus	6.88	kJ/mol	Joback Method
hvap	40.63	kJ/mol	Joback Method
log10ws	-1.54		Crippen Method
logp	1.339		Crippen Method
mcvol	90.630	ml/mol	McGowan Method
pc	5109.34	kPa	Joback Method
rinpol	1071.00		NIST Webbook
rinpol	1106.00		NIST Webbook
rinpol	1090.00		NIST Webbook
rinpol	1071.00		NIST Webbook
rinpol	1071.00		NIST Webbook
rinpol	1072.00		NIST Webbook
rinpol	1071.00		NIST Webbook
rinpol	1102.00		NIST Webbook
rinpol	1103.00		NIST Webbook
rinpol	1090.00		NIST Webbook
rinpol	1072.00		NIST Webbook
rinpol	1098.00		NIST Webbook
rinpol	1103.00		NIST Webbook
ripol	1655.00		NIST Webbook
ripol	1664.00		NIST Webbook
ripol	1664.00		NIST Webbook
ripol	1655.00		NIST Webbook
tb	469.68	K	Joback Method
tc	727.72	K	Joback Method
tf	380.86	K	Joback Method

vc	0.299	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	168.16	J/mol×K	469.68	Joback Method
cpg	178.88	J/mol×K	512.69	Joback Method
cpg	189.07	J/mol×K	555.69	Joback Method
cpg	198.71	J/mol×K	598.70	Joback Method
cpg	207.80	J/mol×K	641.71	Joback Method
cpg	216.33	J/mol×K	684.72	Joback Method
cpg	224.29	J/mol×K	727.72	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=R618296&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
ripol:	Polar retention indices
tb:	Normal Boiling Point Temperature

tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume