

3,5-dimethyl-1,2-dithiolan-4-one

Inchi:	InChI=1S/C5H8OS2/c1-3-5(6)4(2)8-7-3/h3-4H,1-2H3
InchiKey:	DYTKSLFUSUKZJN-UHFFFAOYSA-N
Formula:	C5H8OS2
SMILES:	CC1SSC(C)C1=O
Mol. weight [g/mol]:	148.25

Physical Properties

Property code	Value	Unit	Source
gf	-22.81	kJ/mol	Joback Method
hf	-153.57	kJ/mol	Joback Method
hfus	10.54	kJ/mol	Joback Method
hvap	42.54	kJ/mol	Joback Method
log10ws	-2.07		Crippen Method
logp	1.728		Crippen Method
mcvol	104.720	ml/mol	McGowan Method
pc	4283.05	kPa	Joback Method
rinpol	1124.00		NIST Webbook
rinpol	1134.00		NIST Webbook
rinpol	1115.00		NIST Webbook
rinpol	1115.00		NIST Webbook
rinpol	1098.00		NIST Webbook
rinpol	1098.00		NIST Webbook
rinpol	1111.00		NIST Webbook
rinpol	1124.00		NIST Webbook
ripol	1568.00		NIST Webbook
ripol	1597.00		NIST Webbook
ripol	1568.00		NIST Webbook
tb	487.89	K	Joback Method
tc	740.75	K	Joback Method
tf	387.89	K	Joback Method
vc	0.354	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	209.57	J/mol×K	487.89	Joback Method
cpg	222.26	J/mol×K	530.03	Joback Method
cpg	234.34	J/mol×K	572.18	Joback Method
cpg	245.80	J/mol×K	614.32	Joback Method
cpg	256.62	J/mol×K	656.47	Joback Method
cpg	266.79	J/mol×K	698.61	Joback Method
cpg	276.29	J/mol×K	740.75	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=R235559&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

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