1,2-Dithiolan-4-one, 3,5-dimethyl, #1 (E or Z)

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	1098.00		NIST Webbook
rinpol	1098.00		NIST Webbook
tb	487.89	K	Joback Method
tc	740.75	K	Joback Method
tf	387.89	K	Joback Method
vc	0.354	m3/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

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=R90345&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