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

Inchi: InChI=1S/C6H10OS2/c1-3-5-6(7)4(2)8-9-5/h4-5H,3H2,1-2H3
InchiKey: MMXLOINISPYVFC-UHFFFAOYSA-N
Formula: C6H10OS2
SMILES: CCC1SSC(C)C1=O
Mol. weight [g/mol]: 162.27

Physical Properties

Property code	Value	Unit	Source
gf	-14.39	kJ/mol	Joback Method
hf	-174.21	kJ/mol	Joback Method
hfus	13.13	kJ/mol	Joback Method
hvap	44.77	kJ/mol	Joback Method
log10ws	-2.49		Crippen Method
logp	2.118		Crippen Method
mcvol	118.810	ml/mol	McGowan Method
pc	3791.65	kPa	Joback Method
rinpol	1193.00		NIST Webbook
rinpol	1193.00		NIST Webbook
tb	510.77	K	Joback Method
tc	758.59	K	Joback Method
tf	399.16	K	Joback Method
vc	0.410	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	251.54	J/mol×K	510.77	Joback Method
cpg	265.61	J/mol×K	552.07	Joback Method
cpg	278.98	J/mol×K	593.38	Joback Method
cpg	291.62	J/mol×K	634.68	Joback Method
cpg	303.54	J/mol×K	675.98	Joback Method
cpg	314.72	J/mol×K	717.28	Joback Method
cpg	325.15	J/mol×K	758.59	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R90377&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
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

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