4,5-Thiepanedione, 3,3,6,6-tetramethyl-

Other names: 1,2-Cycloheptanedione-5-thia, 3,3,7,7-tetramethyl-
Inchi: InChI=1S/C10H16O2S/c1-9(2)5-13-6-10(3,4)8(12)7(9)11/h5-6H2,1-4H3
InchiKey: GFZNLWBRSSKIQN-UHFFFAOYSA-N
Formula: C10H16O2S
SMILES: CC1(C)CSCC(C)(C)C(=O)C1=O
Mol. weight [g/mol]: 200.30
CAS: 2800-87-5

Physical Properties

Property code	Value	Unit	Source
gf	-178.34	kJ/mol	Joback Method
hf	-421.57	kJ/mol	Joback Method
hfus	2.54	kJ/mol	Joback Method
hvap	50.15	kJ/mol	Joback Method
ie	8.75	eV	NIST Webbook
log10ws	-1.86		Crippen Method
logp	1.924		Crippen Method
mcvol	160.390	ml/mol	McGowan Method
pc	2995.87	kPa	Joback Method
tb	631.30	K	Joback Method
tc	899.43	K	Joback Method
tf	469.77	K	Joback Method
vc	0.576	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	419.05	J/mol×K	631.30	Joback Method
cpg	438.32	J/mol×K	675.99	Joback Method
cpg	456.77	J/mol×K	720.68	Joback Method
cpg	474.63	J/mol×K	765.37	Joback Method
cpg	492.14	J/mol×K	810.06	Joback Method
cpg	509.52	J/mol×K	854.75	Joback Method
cpg	527.01	J/mol×K	899.43	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=C2800875&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
ie:	Ionization energy
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
pc:	Critical Pressure
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume