3-methyl-2-cyclopentene-1-thione

Other names: 3-methyl-2-cyclopentene-1-thion
Inchi: InChI=1S/C6H8S/c1-5-2-3-6(7)4-5/h4H,2-3H2,1H3
InchiKey: JBWUENDATZQNBX-UHFFFAOYSA-N
Formula: C6H8S
SMILES: CC1=CC(=S)CC1
Mol. weight [g/mol]: 112.19
CAS: 30221-52-4

Physical Properties

Property code	Value	Unit	Source
gf	155.08	kJ/mol	Joback Method
hf	75.06	kJ/mol	Joback Method
hfus	11.03	kJ/mol	Joback Method
hvap	37.95	kJ/mol	Joback Method
log10ws	-2.44		Crippen Method
logp	2.096		Crippen Method
mcvol	92.290	ml/mol	McGowan Method
pc	4468.24	kPa	Joback Method
ripol	1260.00		NIST Webbook
tb	433.41	K	Joback Method
tc	659.63	K	Joback Method
tf	249.47	K	Joback Method
vc	0.338	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	161.65	J/mol×K	433.41	Joback Method
cpg	172.07	J/mol×K	471.11	Joback Method
cpg	181.73	J/mol×K	508.82	Joback Method
cpg	190.70	J/mol×K	546.52	Joback Method
cpg	199.01	J/mol×K	584.23	Joback Method
cpg	206.72	J/mol×K	621.93	Joback Method
cpg	213.90	J/mol×K	659.63	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C30221524&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
ripol:	Polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume