mercaptomethylcyclopentane

Other names: Cyclopentane, mercaptomethyl
Inchi: InChI=1S/C6H12S/c7-5-6-3-1-2-4-6/h6-7H,1-5H2
InchiKey: HBLUJTHFXFVJRN-UHFFFAOYSA-N
Formula: C6H12S
SMILES: SCC1CCCC1
Mol. weight [g/mol]: 116.22

Physical Properties

Property code	Value	Unit	Source
gf	65.58	kJ/mol	Joback Method
hf	-68.21	kJ/mol	Joback Method
hfus	9.27	kJ/mol	Joback Method
hvap	35.94	kJ/mol	Joback Method
log10ws	-2.06		Crippen Method
logp	2.106		Crippen Method
mcvol	100.890	ml/mol	McGowan Method
pc	4162.33	kPa	Joback Method
rinpol	955.00		NIST Webbook
rinpol	957.00		NIST Webbook
rinpol	958.00		NIST Webbook
tb	414.82	K	Joback Method
tc	638.09	K	Joback Method
tf	204.74	K	Joback Method
vc	0.366	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	185.49	J/mol×K	414.82	Joback Method
cpg	200.38	J/mol×K	452.03	Joback Method
cpg	214.40	J/mol×K	489.24	Joback Method
cpg	227.61	J/mol×K	526.45	Joback Method
cpg	240.02	J/mol×K	563.67	Joback Method
cpg	251.67	J/mol×K	600.88	Joback Method

cpg	262.59	J/mol×K	638.09	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R82405&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