1,2-dimercaptocyclopentane

Inchi: InChI=1S/C5H10S2/c6-4-2-1-3-5(4)7/h4-7H,1-3H2
InchiKey: YZVNURZNMBCWGG-UHFFFAOYSA-N
Formula: C5H10S2
SMILES: SC1CCCC1S
Mol. weight [g/mol]: 134.26

Physical Properties

Property code	Value	Unit	Source
gf	78.84	kJ/mol	Joback Method
hf	-29.43	kJ/mol	Joback Method
hfus	11.80	kJ/mol	Joback Method
hvap	40.15	kJ/mol	Joback Method
log10ws	-2.18		Crippen Method
logp	1.767		Crippen Method
mcvol	103.150	ml/mol	McGowan Method
pc	4938.44	kPa	Joback Method
ripol	1520.00		NIST Webbook
ripol	1520.00		NIST Webbook
ripol	1519.00		NIST Webbook
ripol	1519.00		NIST Webbook
tb	450.13	K	Joback Method
tc	704.64	K	Joback Method
tf	225.69	K	Joback Method
vc	0.363	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	193.54	J/mol×K	450.13	Joback Method
cpg	208.03	J/mol×K	492.55	Joback Method
cpg	221.59	J/mol×K	534.97	Joback Method
cpg	234.24	J/mol×K	577.39	Joback Method
cpg	246.03	J/mol×K	619.80	Joback Method
cpg	256.97	J/mol×K	662.22	Joback Method

cpg	267.11	J/mol×K	704.64	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R315754&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

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