1-Mercaptopentan-3-one

Other names: 1-Mercapto-3-pentanone
Inchi: InChI=1S/C5H10OS/c1-2-5(6)3-4-7/h7H,2-4H2,1H3
InchiKey: ORZNCWCHFKUYAZ-UHFFFAOYSA-N
Formula: C5H10OS
SMILES: CCC(=O)CCS
Mol. weight [g/mol]: 118.20

Physical Properties

Property code	Value	Unit	Source
gf	-108.31	kJ/mol	Joback Method
hf	-220.63	kJ/mol	Joback Method
hfus	14.35	kJ/mol	Joback Method
hvap	40.21	kJ/mol	Joback Method
log10ws	-1.27		Crippen Method
logp	1.285		Crippen Method
mcvol	99.230	ml/mol	McGowan Method
pc	4051.80	kPa	Joback Method
rinpol	947.00		NIST Webbook
rinpol	947.00		NIST Webbook
rinpol	947.00		NIST Webbook
rinpol	947.00		NIST Webbook
rinpol	947.00		NIST Webbook
ripol	1517.00		NIST Webbook
ripol	1517.00		NIST Webbook
ripol	1517.00		NIST Webbook
ripol	1517.00		NIST Webbook
tb	430.53	K	Joback Method
tc	633.63	K	Joback Method
tf	232.50	K	Joback Method
vc	0.376	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source

cpg	183.33	J/mol×K	430.53	Joback Method
cpg	192.79	J/mol×K	464.38	Joback Method
cpg	201.83	J/mol×K	498.23	Joback Method
cpg	210.43	J/mol×K	532.08	Joback Method
cpg	218.63	J/mol×K	565.93	Joback Method
cpg	226.42	J/mol×K	599.78	Joback Method
cpg	233.82	J/mol×K	633.63	Joback Method

Sources

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
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=R291960&Units=SI

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
ripol: Polar retention indices
tb: Normal Boiling Point Temperature
tc: Critical Temperature
tf: Normal melting (fusion) point
vc: Critical Volume