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
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

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R603264&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
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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