3-Thia-1-pentanethiol

Inchi: InChI=1S/C4H10S2/c1-2-6-4-3-5/h5H,2-4H2,1H3
InchiKey: IYQVQZXLTJHEKZ-UHFFFAOYSA-N
Formula: C4H10S2
SMILES: CCSCCS
Mol. weight [g/mol]: 122.25

Physical Properties

Property code	Value	Unit	Source
gf	45.31	kJ/mol	Joback Method
hf	-45.54	kJ/mol	Joback Method
hfus	14.29	kJ/mol	Joback Method
hvap	38.05	kJ/mol	Joback Method
log10ws	-1.45		Crippen Method
logp	1.669		Crippen Method
mcvol	99.920	ml/mol	McGowan Method
pc	4322.57	kPa	Joback Method
rinpol	1017.00		NIST Webbook
tb	422.56	K	Joback Method
tc	640.79	K	Joback Method
tf	205.70	K	Joback Method
vc	0.367	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	174.76	J/mol×K	422.56	Joback Method
cpg	184.17	J/mol×K	458.93	Joback Method
cpg	193.17	J/mol×K	495.30	Joback Method
cpg	201.76	J/mol×K	531.68	Joback Method
cpg	209.94	J/mol×K	568.05	Joback Method
cpg	217.72	J/mol×K	604.42	Joback Method
cpg	225.11	J/mol×K	640.79	Joback Method

Sources

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=R156842&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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