4-mercaptononan-2-one

Inchi: InChI=1S/C9H18OS/c1-3-4-5-6-9(11)7-8(2)10/h9,11H,3-7H2,1-2H3
InchiKey: LPWSEWCEKCYPTI-UHFFFAOYSA-N
Formula: C9H18OS
SMILES: CCCCCC(S)CC(C)=O
Mol. weight [g/mol]: 174.30

Physical Properties

Property code	Value	Unit	Source
gf	-77.07	kJ/mol	Joback Method
hf	-308.47	kJ/mol	Joback Method
hfus	21.18	kJ/mol	Joback Method
hvap	48.72	kJ/mol	Joback Method
log10ws	-3.05		Crippen Method
logp	2.844		Crippen Method
mcvol	155.590	ml/mol	McGowan Method
pc	2637.96	kPa	Joback Method
rinpol	1292.00		NIST Webbook
rinpol	1292.00		NIST Webbook
ripol	1802.00		NIST Webbook
tb	521.61	K	Joback Method
tc	719.04	K	Joback Method
tf	262.58	K	Joback Method
vc	0.594	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	350.41	J/mol×K	521.61	Joback Method
cpg	364.73	J/mol×K	554.52	Joback Method
cpg	378.36	J/mol×K	587.42	Joback Method
cpg	391.32	J/mol×K	620.33	Joback Method
cpg	403.62	J/mol×K	653.23	Joback Method
cpg	415.29	J/mol×K	686.14	Joback Method
cpg	426.35	J/mol×K	719.04	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=R292032&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
ripol:	Polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume