3-Mercaptononanal

Inchi: InChI=1S/C9H18OS/c1-2-3-4-5-6-9(11)7-8-10/h8-9,11H,2-7H2,1H3
InchiKey: KCOFYZNOXRYCOE-UHFFFAOYSA-N
Formula: C9H18OS
SMILES: CCCCCCC(S)CC=O
Mol. weight [g/mol]: 174.30

Physical Properties

Property code	Value	Unit	Source
gf	-47.67	kJ/mol	Joback Method
hf	-281.47	kJ/mol	Joback Method
hfus	21.87	kJ/mol	Joback Method
hvap	48.70	kJ/mol	Joback Method
log10ws	-3.05		Crippen Method
logp	2.844		Crippen Method
mcvol	155.590	ml/mol	McGowan Method
pc	2668.02	kPa	Joback Method
rinpol	1320.00		NIST Webbook
tb	516.40	K	Joback Method
tc	709.11	K	Joback Method
tf	254.65	K	Joback Method
vc	0.605	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	351.23	J/mol×K	516.40	Joback Method
cpg	365.20	J/mol×K	548.52	Joback Method
cpg	378.50	J/mol×K	580.64	Joback Method
cpg	391.16	J/mol×K	612.75	Joback Method
cpg	403.19	J/mol×K	644.87	Joback Method
cpg	414.62	J/mol×K	676.99	Joback Method
cpg	425.46	J/mol×K	709.11	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R205593&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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