4-mercaptononan-2-ol

Inchi: InChI=1S/C9H20OS/c1-3-4-5-6-9(11)7-8(2)10/h8-11H,3-7H2,1-2H3
InchiKey: FRCYEBKGSWZYRK-UHFFFAOYSA-N
Formula: C9H20OS
SMILES: CCCCCC(S)CC(C)O
Mol. weight [g/mol]: 176.32

Physical Properties

Property code	Value	Unit	Source
gf	-87.41	kJ/mol	Joback Method
hf	-353.40	kJ/mol	Joback Method
hfus	20.15	kJ/mol	Joback Method
hvap	58.27	kJ/mol	Joback Method
log10ws	-3.15		Crippen Method
logp	2.636		Crippen Method
mcvol	159.890	ml/mol	McGowan Method
pc	2741.15	kPa	Joback Method
rinpol	1323.00		NIST Webbook
rinpol	1315.00		NIST Webbook
ripol	1971.00		NIST Webbook
ripol	1985.00		NIST Webbook
tb	559.48	K	Joback Method
tc	741.62	K	Joback Method
tf	258.47	K	Joback Method
vc	0.601	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	387.91	J/mol×K	559.48	Joback Method
cpg	401.20	J/mol×K	589.84	Joback Method
cpg	413.88	J/mol×K	620.19	Joback Method
cpg	425.98	J/mol×K	650.55	Joback Method
cpg	437.50	J/mol×K	680.90	Joback Method
cpg	448.47	J/mol×K	711.26	Joback Method

cpg	458.91	J/mol×K	741.62	Joback Method

Sources

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=R291920&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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