Octanamide, N-(2-mercaptoethyl)-

Other names: N-(2-Mercaptoethyl) octanamide
Inchi: InChI=1S/C10H21NOS/c1-2-3-4-5-6-7-10(12)11-8-9-13/h13H,2-9H2,1H3,(H,11,12)
InchiKey: JLZORHOCSVVPHT-UHFFFAOYSA-N
Formula: C10H21NOS
SMILES: CCCCCCCC(=O)NCCS
Mol. weight [g/mol]: 203.34
CAS: 56630-30-9

Physical Properties

Property code	Value	Unit	Source
gf	23.18	kJ/mol	Joback Method
hf	-270.36	kJ/mol	Joback Method
hfus	32.40	kJ/mol	Joback Method
hvap	57.77	kJ/mol	Joback Method
log10ws	-3.05		Crippen Method
logp	2.393		Crippen Method
mcvol	179.660	ml/mol	McGowan Method
pc	2407.64	kPa	Joback Method
tb	595.10	K	Joback Method
tc	787.17	K	Joback Method
tf	341.51	K	Joback Method
vc	0.691	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	448.85	J/mol×K	595.10	Joback Method
cpg	463.52	J/mol×K	627.11	Joback Method
cpg	477.46	J/mol×K	659.12	Joback Method
cpg	490.69	J/mol×K	691.14	Joback Method
cpg	503.24	J/mol×K	723.15	Joback Method
cpg	515.13	J/mol×K	755.16	Joback Method
cpg	526.37	J/mol×K	787.17	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=C56630309&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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume