Aminothioacetic acid

Inchi: InChI=1S/C2H5NOS/c3-1-2(4)5/h1,3H2,(H,4,5)
InchiKey: CYFJIBWZIQDUSZ-UHFFFAOYSA-N
Formula: C2H5NOS
SMILES: NCC(=O)S
Mol. weight [g/mol]: 91.13
CAS: 758-10-1

Physical Properties

Property code	Value	Unit	Source
gf	-67.12	kJ/mol	Joback Method
hf	-124.92	kJ/mol	Joback Method
hfus	11.77	kJ/mol	Joback Method
hvap	44.17	kJ/mol	Joback Method
log10ws	0.06		Crippen Method
logp	-0.599		Crippen Method
mcvol	66.940	ml/mol	McGowan Method
pc	6653.02	kPa	Joback Method
tb	434.42	K	Joback Method
tc	659.97	K	Joback Method
tf	281.95	K	Joback Method
vc	0.236	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	117.31	J/mol×K	434.42	Joback Method
cpg	122.86	J/mol×K	472.01	Joback Method
cpg	128.12	J/mol×K	509.60	Joback Method
cpg	133.10	J/mol×K	547.19	Joback Method
cpg	137.79	J/mol×K	584.79	Joback Method
cpg	142.21	J/mol×K	622.38	Joback Method
cpg	146.36	J/mol×K	659.97	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=C758101&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

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