

DL-alpha-aminothiopropionic acid

Inchi:	InChI=1S/C3H7NOS/c1-2(4)3(5)6/h2H,4H2,1H3,(H,5,6)
InchiKey:	YXXURDJTDAAEPH-UHFFFAOYSA-N
Formula:	C3H7NOS
SMILES:	CC(N)C(=O)S
Mol. weight [g/mol]:	105.16
CAS:	758-28-1

Physical Properties

Property code	Value	Unit	Source
gf	-61.14	kJ/mol	Joback Method
hf	-150.84	kJ/mol	Joback Method
hfus	10.84	kJ/mol	Joback Method
hvap	46.01	kJ/mol	Joback Method
log10ws	-0.47		Crippen Method
logp	-0.210		Crippen Method
mcvol	81.030	ml/mol	McGowan Method
pc	5791.74	kPa	Joback Method
tb	456.86	K	Joback Method
tc	684.59	K	Joback Method
tf	278.22	K	Joback Method
vc	0.286	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	153.24	J/molxK	456.86	Joback Method
cpg	160.71	J/molxK	494.82	Joback Method
cpg	167.77	J/molxK	532.77	Joback Method
cpg	174.43	J/molxK	570.73	Joback Method
cpg	180.70	J/molxK	608.68	Joback Method
cpg	186.58	J/molxK	646.64	Joback Method
cpg	192.10	J/molxK	684.59	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C758281&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307I
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

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
mccvol:	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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