Thiosulfuric acid, s-(2-amino-2,3-dimethylbutyl) ester

Inchi: InChI=1S/C6H15NO3S2/c1-5(2)6(3,7)4-11-12(8,9)10/h5H,4,7H2,1-3H3,(H,8,9,10)
InchiKey: DCHHOPWXFOJUML-UHFFFAOYSA-N
Formula: C6H15NO3S2
SMILES: CC(C)C(C)(N)CSS(=O)(=O)O
Mol. weight [g/mol]: 213.32
CAS: 13893-05-5

Physical Properties

Property code	Value	Unit	Source
gf	-505.75	kJ/mol	Joback Method
hf	-711.12	kJ/mol	Joback Method
hfus	25.15	kJ/mol	Joback Method
hvap	80.04	kJ/mol	Joback Method
log10ws	-1.66		Crippen Method
logp	0.896		Crippen Method
mcvol	155.690	ml/mol	McGowan Method
pc	4782.59	kPa	Joback Method
tb	614.28	K	Joback Method
tc	812.97	K	Joback Method
tf	361.84	K	Joback Method
vc	0.583	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	391.55	J/mol×K	614.28	Joback Method
cpg	402.83	J/mol×K	647.40	Joback Method
cpg	413.40	J/mol×K	680.51	Joback Method
cpg	423.27	J/mol×K	713.63	Joback Method
cpg	432.45	J/mol×K	746.74	Joback Method
cpg	440.96	J/mol×K	779.86	Joback Method
cpg	448.80	J/mol×K	812.97	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=C13893055&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