Thiosulfuric acid,s-(2-amino-2-methylpentyl)ester

Inchi: InChI=1S/C6H15NO3S2/c1-3-4-6(2,7)5-11-12(8,9)10/h3-5,7H2,1-2H3,(H,8,9,10)
InchiKey: KROQVRDOMZSPND-UHFFFAOYSA-N
Formula: C6H15NO3S2
SMILES: CCCC(C)(N)CSS(=O)(=O)O
Mol. weight [g/mol]: 213.32
CAS: 13893-04-4

Physical Properties

Property code	Value	Unit	Source
gf	-503.31	kJ/mol	Joback Method
hf	-705.84	kJ/mol	Joback Method
hfus	28.68	kJ/mol	Joback Method
hvap	80.43	kJ/mol	Joback Method
log10ws	-1.90		Crippen Method
logp	1.040		Crippen Method
mcvol	155.690	ml/mol	McGowan Method
pc	4730.11	kPa	Joback Method
tb	614.72	K	Joback Method
tc	809.74	K	Joback Method
tf	376.84	K	Joback Method
vc	0.589	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	391.07	J/mol×K	614.72	Joback Method
cpg	402.10	J/mol×K	647.22	Joback Method
cpg	412.45	J/mol×K	679.73	Joback Method
cpg	422.14	J/mol×K	712.23	Joback Method
cpg	431.17	J/mol×K	744.73	Joback Method
cpg	439.56	J/mol×K	777.24	Joback Method
cpg	447.32	J/mol×K	809.74	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C13893044&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Joback Method:	https://en.wikipedia.org/wiki/Joback_method

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