DL-Homocysteine, S-ethyl-

Other names:	Butyric acid, 2-amino-4-(ethylthio)-, DL- (.+/-.)-Ethionine Aethionin CN 8676 DL-Ethionine DL-2-Amino-4-(ethylthio)butyric acid Ethionin Ethionine NSC-751 Butyric acid, DL-2-amino-4-(ethylthio)- Ethionine, DL- U-1434 2-Amino-4-(ethylthio)butyric acid Homocysteine, S-ethyl- S-Ethyl-DL-homocysteine
Inchi:	InChI=1S/C6H13NO2S/c1-2-10-4-3-5(7)6(8)9/h5H,2-4,7H2,1H3,(H,8,9)
InchiKey:	GGLZPLKKBSSKCX-UHFFFAOYSA-N
Formula:	C6H13NO2S
SMILES:	CCSCCC(N)C(=O)O
Mol. weight [g/mol]:	163.24
CAS:	67-21-0

Physical Properties

Property code	Value	Unit	Source
gf	-168.97	kJ/mol	Joback Method
hf	-361.60	kJ/mol	Joback Method
hfus	22.79	kJ/mol	Joback Method
hvap	69.44	kJ/mol	Joback Method
log10ws	-0.86		Crippen Method
logp	0.542		Crippen Method
mcvol	129.170	ml/mol	McGowan Method
pc	4124.99	kPa	Joback Method
tb	623.60	K	Joback Method
tc	825.09	K	Joback Method
tf	370.79	K	Joback Method
vc	0.473	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	320.77	J/mol×K	623.60	Joback Method
cpg	330.35	J/mol×K	657.18	Joback Method
cpg	339.40	J/mol×K	690.76	Joback Method
cpg	347.93	J/mol×K	724.34	Joback Method
cpg	355.96	J/mol×K	757.93	Joback Method
cpg	363.48	J/mol×K	791.51	Joback Method
cpg	370.52	J/mol×K	825.09	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=C67210&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