HOMOSERINE

Other names: Butyric acid, 2-amino-4-hydroxy-, DL-
Inchi: InChI=1S/C4H9NO3/c5-3(1-2-6)4(7)8/h3,6H,1-2,5H2,(H,7,8)
InchiKey: UKAUYVFTDYCKQA-UHFFFAOYSA-N
Formula: C4H9NO3
SMILES: NC(CCO)C(=O)O
Mol. weight [g/mol]: 119.12

Physical Properties

Property code	Value	Unit	Source
hf	-597.48	kJ/mol	Cheméo Relay (1.0)
hfus	17.57	kJ/mol	Joback Method
ie	9.16	eV	Cheméo Relay (1.0)
log10ws	0.54		Cheméo Relay (1.0)
logp	-1.219		Crippen Method
mcvol	90.510	ml/mol	McGowan Method
tf	486.11	K	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	227.94	J/mol×K	601.24	Joback Method
cpg	234.21	J/mol×K	631.28	Joback Method
cpg	240.18	J/mol×K	661.32	Joback Method
cpg	245.83	J/mol×K	691.36	Joback Method
cpg	251.20	J/mol×K	721.39	Joback Method
cpg	256.27	J/mol×K	751.43	Joback Method
cpg	261.07	J/mol×K	781.47	Joback Method

Sources

McGowan Method: http://link.springer.com/article/10.1007/BF02311772

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Cheméo Relay (1.0):	
Cheméo Relay (1.0, beta):	
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C1927259&Units=SI
Joback Method:	https://en.wikipedia.org/wiki/Joback_method

Legend

cpg:	Ideal gas heat capacity
hf:	Enthalpy of formation at standard conditions
hfus:	Enthalpy of fusion at standard conditions
ie:	Ionization energy
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
tf:	Normal melting (fusion) point