3,3'-Iminodipropionic acid

Other names: N-(2-carboxyethyl)-«beta»-alanine
Inchi: InChI=1S/C6H11NO4/c8-5(9)1-3-7-4-2-6(10)11/h7H,1-4H2,(H,8,9)(H,10,11)
InchiKey: TXPKUUXHNFRBPS-UHFFFAOYSA-N
Formula: C6H11NO4
SMILES: O=C(O)CCNCCC(=O)O
Mol. weight [g/mol]: 161.16
CAS: 505-47-5

Physical Properties

Property code	Value	Unit	Source
gf	-442.45	kJ/mol	Joback Method
hf	-643.32	kJ/mol	Joback Method
hfus	27.77	kJ/mol	Joback Method
hvap	82.24	kJ/mol	Joback Method
log10ws	0.28		Crippen Method
logp	-0.475		Crippen Method
mcvol	120.260	ml/mol	McGowan Method
pc	4621.41	kPa	Joback Method
tb	678.95	K	Joback Method
tc	855.82	K	Joback Method
tf	431.54	K	Joback Method
vc	0.457	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	320.91	J/mol×K	678.95	Joback Method
cpg	328.18	J/mol×K	708.43	Joback Method
cpg	335.06	J/mol×K	737.91	Joback Method
cpg	341.57	J/mol×K	767.38	Joback Method
cpg	347.72	J/mol×K	796.86	Joback Method
cpg	353.52	J/mol×K	826.34	Joback Method
cpg	358.98	J/mol×K	855.82	Joback Method

Sources

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=C505475&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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