1-Propanol, 2-amino-, (S)-

Other names: 2-Amino-1-propanol
(S)-(+)-2-Amino-1-propanol
(+)-2-aminopropan-1-ol
Inchi: InChI=1S/C3H9NO/c1-3(4)2-5/h3,5H,2,4H2,1H3/t3-/m1/s1
InchiKey: BKMMTJMQCTUHRP-GSVOUGTGSA-N
Formula: C3H9NO
SMILES: CC(N)CO
Mol. weight [g/mol]: 75.11
CAS: 2749-11-3

Physical Properties

Property code	Value	Unit	Source
gf	-98.43	kJ/mol	Joback Method
hf	-228.97	kJ/mol	Joback Method
hfus	9.29	kJ/mol	Joback Method
hvap	49.20	kJ/mol	Joback Method
log10ws	0.11		Crippen Method
logp	-0.674		Crippen Method
mcvol	68.980	ml/mol	McGowan Method
pc	5495.11	kPa	Joback Method
tb	432.31	K	Joback Method
tc	613.40	K	Joback Method
tf	252.65	K	Joback Method
vc	0.245	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	142.31	J/mol×K	432.31	Joback Method
cpg	149.06	J/mol×K	462.49	Joback Method
cpg	155.54	J/mol×K	492.67	Joback Method
cpg	161.74	J/mol×K	522.85	Joback Method
cpg	167.68	J/mol×K	553.03	Joback Method
cpg	173.36	J/mol×K	583.21	Joback Method

cpg	178.78	J/mol×K	613.40	Joback Method

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	345.70	K	1.50	NIST Webbook

Sources

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
McGowan Method: http://link.springer.com/article/10.1007/BF02311772
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C2749113&Units=SI

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
tbrp: Boiling point at reduced pressure
tc: Critical Temperature
tf: Normal melting (fusion) point
vc: Critical Volume

Cheméo (https://www.chemeo.com) is the biggest free database of chemical and physical data for the process industry.