2-amino-4-methylpentan-1-ol

Other names: 1-Pentanol, 2-amino-4-methyl-
Inchi: InChI=1S/C6H15NO/c1-5(2)3-6(7)4-8/h5-6,8H,3-4,7H2,1-2H3
InchiKey: VPSSPAXIFBTOHY-UHFFFAOYSA-N
Formula: C6H15NO
SMILES: CC(C)CC(N)CO
Mol. weight [g/mol]: 117.19
CAS: 502-32-9

Physical Properties

Property code	Value	Unit	Source
gf	-75.61	kJ/mol	Joback Method
hf	-296.17	kJ/mol	Joback Method
hfus	13.53	kJ/mol	Joback Method
hvap	55.49	kJ/mol	Joback Method
log10ws	-0.90		Crippen Method
logp	0.352		Crippen Method
mcvol	111.250	ml/mol	McGowan Method
pc	3768.41	kPa	Joback Method
tb	500.51	K	Joback Method
tc	680.59	K	Joback Method
tf	271.46	K	Joback Method
vc	0.407	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	261.10	J/mol×K	500.51	Joback Method
cpg	271.63	J/mol×K	530.52	Joback Method
cpg	281.69	J/mol×K	560.54	Joback Method
cpg	291.31	J/mol×K	590.55	Joback Method
cpg	300.49	J/mol×K	620.56	Joback Method
cpg	309.25	J/mol×K	650.57	Joback Method
cpg	317.61	J/mol×K	680.59	Joback Method

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	371.50 ± 0.50	K	1.50	NIST Webbook

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=C502329&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
tbrp:	Boiling point at reduced pressure
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume