

2-Methylbutylglycine

Inchi:	InChI=1S/C7H15NO2/c1-3-5(2)4-6(8)7(9)10/h5-6H,3-4,8H2,1-2H3,(H,9,10)
InchiKey:	MBZXSJWDBIIBLL-UHFFFAOYSA-N
Formula:	C7H15NO2
SMILES:	CCC(C)CC(N)C(=O)O
Mol. weight [g/mol]:	145.20
CAS:	3570-21-6

Physical Properties

Property code	Value	Unit	Source
gf	-196.11	kJ/mol	Joback Method
hf	-429.39	kJ/mol	Joback Method
hfus	17.72	kJ/mol	Joback Method
hvap	64.47	kJ/mol	Joback Method
log10ws	-1.16		Crippen Method
logp	0.835		Crippen Method
mcvol	126.910	ml/mol	McGowan Method
pc	3620.24	kPa	Joback Method
tb	577.26	K	Joback Method
tc	763.93	K	Joback Method
tf	332.66	K	Joback Method
vc	0.469	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	320.89	J/molxK	577.26	Joback Method
cpg	331.46	J/molxK	608.37	Joback Method
cpg	341.51	J/molxK	639.48	Joback Method
cpg	351.06	J/molxK	670.59	Joback Method
cpg	360.12	J/molxK	701.70	Joback Method
cpg	368.71	J/molxK	732.82	Joback Method
cpg	376.84	J/molxK	763.93	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=C3570216&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071

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
hvac:	Enthalpy of vaporization at standard conditions
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mccol:	McGowan's characteristic volume
pc:	Critical Pressure
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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