(3-Methylbut-2-yl) glycine

Inchi: InChI=1S/C7H15NO2/c1-4(2)5(3)6(8)7(9)10/h4-6H,8H2,1-3H3,(H,9,10)
InchiKey: VFEDCKXLINRKLV-UHFFFAOYSA-N
Formula: C7H15NO2
SMILES: CC(C)C(C)C(N)C(=O)O
Mol. weight [g/mol]: 145.20
CAS: 19531-09-0

Physical Properties

Property code	Value	Unit	Source
gf	-198.55	kJ/mol	Joback Method
hf	-434.67	kJ/mol	Joback Method
hfus	14.20	kJ/mol	Joback Method
hvap	64.08	kJ/mol	Joback Method
log10ws	-0.91		Crippen Method
logp	0.690		Crippen Method
mcvol	126.910	ml/mol	McGowan Method
pc	3655.35	kPa	Joback Method
tb	576.82	K	Joback Method
tc	767.06	K	Joback Method
tf	317.66	K	Joback Method
vc	0.464	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	321.31	J/mol×K	576.82	Joback Method
cpg	332.13	J/mol×K	608.53	Joback Method
cpg	342.41	J/mol×K	640.23	Joback Method
cpg	352.16	J/mol×K	671.94	Joback Method
cpg	361.40	J/mol×K	703.65	Joback Method
cpg	370.13	J/mol×K	735.36	Joback Method
cpg	378.39	J/mol×K	767.06	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=C19531090&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