Isobutyrylglycine, methyl ester

Inchi: InChI=1S/C7H13NO3/c1-5(2)7(10)8-4-6(9)11-3/h5H,4H2,1-3H3,(H,8,10)
InchiKey: NZZLARRIBIFCBC-UHFFFAOYSA-N
Formula: C7H13NO3
SMILES: COC(=O)CNC(=O)C(C)C
Mol. weight [g/mol]: 159.18

Physical Properties

Property code	Value	Unit	Source
gf	-267.83	kJ/mol	Joback Method
hf	-497.00	kJ/mol	Joback Method
hfus	19.85	kJ/mol	Joback Method
hvap	53.13	kJ/mol	Joback Method
log10ws	-0.34		Crippen Method
logp	-0.068		Crippen Method
mcvol	128.480	ml/mol	McGowan Method
pc	3228.31	kPa	Joback Method
rinpol	1207.00		NIST Webbook
rinpol	1207.00		NIST Webbook
tb	539.45	K	Joback Method
tc	732.01	K	Joback Method
tf	328.40	K	Joback Method
vc	0.486	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	300.32	J/mol×K	539.45	Joback Method
cpg	311.59	J/mol×K	571.54	Joback Method
cpg	322.35	J/mol×K	603.64	Joback Method
cpg	332.61	J/mol×K	635.73	Joback Method
cpg	342.37	J/mol×K	667.82	Joback Method
cpg	351.63	J/mol×K	699.92	Joback Method
cpg	360.39	J/mol×K	732.01	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=R245551&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
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume