Isovalerylglycine, methyl ester

Inchi: InChI=1S/C9H17NO3/c1-7(2)4-5-8(11)10-6-9(12)13-3/h7H,4-6H2,1-3H3,(H,10,11)
InchiKey: QTWNOLOFZKGWMY-UHFFFAOYSA-N
Formula: C9H17NO3
SMILES: COC(=O)CNC(=O)CCC(C)C
Mol. weight [g/mol]: 187.24

Physical Properties

Property code	Value	Unit	Source
gf	-250.99	kJ/mol	Joback Method
hf	-538.28	kJ/mol	Joback Method
hfus	25.03	kJ/mol	Joback Method
hvap	57.58	kJ/mol	Joback Method
log10ws	-1.18		Crippen Method
logp	0.712		Crippen Method
mcvol	156.660	ml/mol	McGowan Method
pc	2624.46	kPa	Joback Method
rinpol	1308.00		NIST Webbook
rinpol	1308.00		NIST Webbook
tb	585.21	K	Joback Method
tc	773.19	K	Joback Method
tf	350.94	K	Joback Method
vc	0.599	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	393.11	J/mol×K	585.21	Joback Method
cpg	406.08	J/mol×K	616.54	Joback Method
cpg	418.44	J/mol×K	647.87	Joback Method
cpg	430.20	J/mol×K	679.20	Joback Method
cpg	441.37	J/mol×K	710.53	Joback Method
cpg	451.95	J/mol×K	741.86	Joback Method
cpg	461.96	J/mol×K	773.19	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=R245566&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