N-Formyl-dl-leucine

Other names: DL-Leucine, N-formyl-
Inchi: InChI=1S/C7H13NO3/c1-5(2)3-6(7(10)11)8-4-9/h4-6H,3H2,1-2H3,(H,8,9)(H,10,11)
InchiKey: HFBHOAHFRNLZGN-UHFFFAOYSA-N
Formula: C7H13NO3
SMILES: CC(C)CC(NC=O)C(=O)O
Mol. weight [g/mol]: 159.18
CAS: 5338-45-4

Physical Properties

Property code	Value	Unit	Source
chs	-3841.60 ± 0.30	kJ/mol	NIST Webbook
gf	-272.69	kJ/mol	Joback Method
hf	-495.29	kJ/mol	Joback Method
hfus	19.92	kJ/mol	Joback Method
hvap	66.98	kJ/mol	Joback Method
log10ws	-0.69		Crippen Method
logp	0.232		Crippen Method
mcvol	128.480	ml/mol	McGowan Method
pc	3754.57	kPa	Joback Method
tb	603.56	K	Joback Method
tc	786.88	K	Joback Method
tf	344.06	K	Joback Method
vc	0.492	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	326.88	J/mol×K	603.56	Joback Method
cpg	336.47	J/mol×K	634.11	Joback Method
cpg	345.56	J/mol×K	664.67	Joback Method
cpg	354.18	J/mol×K	695.22	Joback Method
cpg	362.33	J/mol×K	725.77	Joback Method
cpg	370.03	J/mol×K	756.32	Joback Method
cpg	377.29	J/mol×K	786.88	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=C5338454&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

Legend

chs:	Standard solid enthalpy of combustion
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