L-Isoleucine

Other names:	Isoleucine, L- «alpha»-Amino-«beta»-methylvaleric acid, (2S,3S)- Acetic acid, amino(1-methylpropyl)-, (R*,R*)- L-(+)-Isoleucine L-Norvaline, 3-methyl-, erythro- Norvaline, 3-methyl-, erythro- Pentanoic acid, 2-amino-3-methyl-, (2S,3S)- Pentanoic acid, 2-amino-3-methyl-, [S-(R*,R*)]- Valeric acid, 2-amino-3-methyl- 2-Amino-3-methylpentanoic acid, (S-(R*,R*))- 2-Amino-3-methylvaleric acid sec-C4H9CH(NH2)COOH Acetic acid, amino-sec-butyl- [S-(R*,R*)]-2-Amino-3-methylpentanoic acid (2S,3S)-2-Amino-3-methylpentanoic acid (2S,3S)-«alpha»-Amino-«beta»-methyl-n-valeric acid (S)-Isoleucine (S,S)-Isoleucine 2S,3S-Isoleucine L-Ile Isoleucine NSC 46708
Inchi:	InChI=1S/C6H13NO2/c1-3-4(2)5(7)6(8)9/h4-5H,3,7H2,1-2H3,(H,8,9)/t4-,5+/m0/s1
InchiKey:	AGPKZVBTJJNPAG-CRCLSJGQSA-N
Formula:	C6H13NO2
SMILES:	CCC(C)C(N)C(=O)O
Mol. weight [g/mol]:	131.17
CAS:	73-32-5

Physical Properties

Property code	Value	Unit	Source
affp	923.40	kJ/mol	NIST Webbook
affp	917.40	kJ/mol	NIST Webbook
basg	883.50	kJ/mol	NIST Webbook
chs	-3578.30 ± 1.40	kJ/mol	NIST Webbook
chs	-3572.00 ± 0.30	kJ/mol	NIST Webbook

gf	-204.53	kJ/mol	Joback Method
hf	-408.75	kJ/mol	Joback Method
hfs	-640.60 ± 1.90	kJ/mol	NIST Webbook
hfs	-638.10	kJ/mol	NIST Webbook
hfus	15.13	kJ/mol	Joback Method
hvap	62.24	kJ/mol	Joback Method
ie	8.66	eV	NIST Webbook
ie	9.50 ± 0.20	eV	NIST Webbook
log10ws	-0.74		Crippen Method
logp	0.444		Crippen Method
mcvol	112.820	ml/mol	McGowan Method
pc	4077.71	kPa	Joback Method
ss	207.99	J/mol×K	NIST Webbook
tb	554.38	K	Joback Method
tc	743.19	K	Joback Method
tf	321.39	K	Joback Method
vc	0.413	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	311.64	J/mol×K	680.26	Joback Method
cpg	319.50	J/mol×K	711.72	Joback Method
cpg	275.71	J/mol×K	554.38	Joback Method
cpg	285.39	J/mol×K	585.85	Joback Method
cpg	294.59	J/mol×K	617.32	Joback Method
cpg	303.34	J/mol×K	648.79	Joback Method
cpg	326.94	J/mol×K	743.19	Joback Method
cps	188.28	J/mol×K	298.15	NIST Webbook
hsubt	120.00 ± 0.80	kJ/mol	455.00	NIST Webbook

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C73325&Units=SI

Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

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

Legend

affp:	Proton affinity
basg:	Gas basicity
chs:	Standard solid enthalpy of combustion
cpg:	Ideal gas heat capacity
cps:	Solid phase heat capacity
gf:	Standard Gibbs free energy of formation
hf:	Enthalpy of formation at standard conditions
hfs:	Solid phase enthalpy of formation at standard conditions
hfus:	Enthalpy of fusion at standard conditions
hsubt:	Enthalpy of sublimation at a given temperature
hvap:	Enthalpy of vaporization at standard conditions
ie:	Ionization energy
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
pc:	Critical Pressure
ss:	Solid phase molar entropy at standard conditions
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume