

DL-Isoleucine

Other names:	Isoleucine, DL- DL-allo-isoleucine
Inchi:	InChI=1S/C6H13NO2/c1-3-4(2)5(7)6(8)9/h4-5H,3,7H2,1-2H3,(H,8,9)
InchiKey:	AGPKZVBTJJNPAG-UHFFFAOYSA-N
Formula:	C6H13NO2
SMILES:	CCC(C)C(N)C(=O)O
Mol. weight [g/mol]:	131.17
CAS:	443-79-8

Physical Properties

Property code	Value	Unit	Source
chs	-3583.70 ± 1.80	kJ/mol	NIST Webbook
chs	-3583.70 ± 1.90	kJ/mol	NIST Webbook
gf	-204.53	kJ/mol	Joback Method
hf	-408.75	kJ/mol	Joback Method
hfs	-635.20 ± 1.90	kJ/mol	NIST Webbook
hfus	15.13	kJ/mol	Joback Method
hvap	62.24	kJ/mol	Joback Method
log10ws	-0.74		Crippen Method
logp	0.444		Crippen Method
mcvol	112.820	ml/mol	McGowan Method
pc	4077.71	kPa	Joback Method
tb	554.38	K	Joback Method
tc	743.19	K	Joback Method
tf	321.39	K	Joback Method
vc	0.413	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
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	311.64	J/mol×K	680.26	Joback Method
cpg	319.50	J/mol×K	711.72	Joback Method
cpg	326.94	J/mol×K	743.19	Joback Method

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
Crippen Method:	https://www.cheméo.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=C443798&Units=SI

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
hfs:	Solid phase 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

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