

N-Acetyl-D-leucine amide

Inchi:	InChI=1S/C8H16N2O2/c1-5(2)4-7(8(9)12)10-6(3)11/h5,7H,4H2,1-3H3,(H2,9,12)(H,10,11)
InchiKey:	PHPXQAHAQREGGN-SSDOTTSWSA-N
Formula:	C8H16N2O2
SMILES:	CC(=O)NC(CC(C)C)C(N)=O
Mol. weight [g/mol]:	172.22
CAS:	16624-68-3

Physical Properties

Property code	Value	Unit	Source
gf	-90.40	kJ/mol	Joback Method
hf	-356.91	kJ/mol	Joback Method
hfus	22.92	kJ/mol	Joback Method
hsub	120.40 ± 0.40	kJ/mol	NIST Webbook
hvap	63.19	kJ/mol	Joback Method
log10ws	-1.22		Crippen Method
logp	0.023		Crippen Method
mcvol	146.680	ml/mol	McGowan Method
pc	3177.55	kPa	Joback Method
tb	612.00	K	Joback Method
tc	816.13	K	Joback Method
tf	385.70	K	Joback Method
vc	0.547	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	380.07	J/mol×K	612.00	Joback Method
cpg	435.49	J/mol×K	782.11	Joback Method
cpg	425.74	J/mol×K	748.09	Joback Method
cpg	415.34	J/mol×K	714.06	Joback Method
cpg	404.28	J/mol×K	680.04	Joback Method
cpg	392.53	J/mol×K	646.02	Joback Method
cpg	444.62	J/mol×K	816.13	Joback Method
hfust	20.20	kJ/mol	404.00	NIST Webbook

hfust	20.20	kJ/mol	404.00	NIST Webbook
hfust	20.20	kJ/mol	404.00	NIST Webbook
hsubt	101.00 ± 3.00	kJ/mol	387.50	NIST Webbook
hsubt	114.80 ± 0.30	kJ/mol	393.00	NIST Webbook
sfust	50.00	J/mol×K	404.00	NIST Webbook

Sources

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=C16624683&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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
hfust:	Enthalpy of fusion at a given temperature
hsub:	Enthalpy of sublimation at standard conditions
hsubt:	Enthalpy of sublimation at a given temperature
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
sfust:	Entropy of fusion at a given temperature
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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