

# Glutamine, n-isopropyl-

<b>Inchi:</b>	InChI=1S/C8H16N2O3/c1-5(2)10-7(11)4-3-6(9)8(12)13/h5-6H,3-4,9H2,1-2H3,(H,10,11)(H,12)
<b>InchiKey:</b>	CABXGBMKSVRWOG-UHFFFAOYSA-N
<b>Formula:</b>	C8H16N2O3
<b>SMILES:</b>	CC(C)NC(=O)CCC(N)C(=O)O
<b>Mol. weight [g/mol]:</b>	188.22

## Physical Properties

Property code	Value	Unit	Source
gf	-227.22	kJ/mol	Joback Method
hf	-509.14	kJ/mol	Joback Method
hfus	27.01	kJ/mol	Joback Method
hvap	79.87	kJ/mol	Joback Method
log10ws	-0.89		Crippen Method
logp	-0.297		Crippen Method
mcvol	152.550	ml/mol	McGowan Method
pc	3534.66	kPa	Joback Method
tb	704.18	K	Joback Method
tc	897.64	K	Joback Method
tf	446.52	K	Joback Method
vc	0.567	m3/kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	429.76	J/molxK	704.18	Joback Method
cpg	439.99	J/molxK	736.42	Joback Method
cpg	449.61	J/molxK	768.67	Joback Method
cpg	458.65	J/molxK	800.91	Joback Method
cpg	467.13	J/molxK	833.15	Joback Method
cpg	475.06	J/molxK	865.40	Joback Method
cpg	482.46	J/molxK	897.64	Joback Method

# Sources

<b>Joback Method:</b>	<a href="https://en.wikipedia.org/wiki/Joback_method">https://en.wikipedia.org/wiki/Joback_method</a>
<b>McGowan Method:</b>	<a href="http://link.springer.com/article/10.1007/BF02311772">http://link.springer.com/article/10.1007/BF02311772</a>
<b>NIST Webbook:</b>	<a href="http://webbook.nist.gov/cgi/cbook.cgi?ID=B6007417&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=B6007417&amp;Units=SI</a>
<b>Crippen Method:</b>	<a href="http://pubs.acs.org/doi/abs/10.1021/ci990307l">http://pubs.acs.org/doi/abs/10.1021/ci990307l</a>
<b>Crippen Method:</b>	<a href="https://www.chemeo.com/doc/models/crippen_log10ws">https://www.chemeo.com/doc/models/crippen_log10ws</a>

# Legend

<b>cpg:</b>	Ideal gas heat capacity
<b>gf:</b>	Standard Gibbs free energy of formation
<b>hf:</b>	Enthalpy of formation at standard conditions
<b>hfus:</b>	Enthalpy of fusion at standard conditions
<b>hvap:</b>	Enthalpy of vaporization at standard conditions
<b>log10ws:</b>	Log10 of Water solubility in mol/l
<b>logp:</b>	Octanol/Water partition coefficient
<b>mcvol:</b>	McGowan's characteristic volume
<b>pc:</b>	Critical Pressure
<b>tb:</b>	Normal Boiling Point Temperature
<b>tc:</b>	Critical Temperature
<b>tf:</b>	Normal melting (fusion) point
<b>vc:</b>	Critical Volume

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