

N-isobutylurea

Inchi:	InChI=1S/C5H12N2O/c1-4(2)3-7-5(6)8/h4H,3H2,1-2H3,(H3,6,7,8)
InchiKey:	MQBITTBZTXUIPN-UHFFFAOYSA-N
Formula:	C5H12N2O
SMILES:	CC(C)CNC(=N)O
Mol. weight [g/mol]:	116.16
CAS:	592-17-6

Physical Properties

Property code	Value	Unit	Source
gf	144.95	kJ/mol	Joback Method
hf	-52.24	kJ/mol	Joback Method
hvap	61.53	kJ/mol	Joback Method
log10ws	-2.09		Crippen Method
logp	0.725		Crippen Method
mcvol	102.840	ml/mol	McGowan Method
tb	540.05	K	Joback Method
tf	313.37	K	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	244.79	J/molxK	540.05	Joback Method
cpg	45.27	J/molxK	100.12	Joback Method
cpg	45.27	J/molxK	100.12	Joback Method
cpg	45.27	J/molxK	100.12	Joback Method
cpg	45.27	J/molxK	100.12	Joback Method
cpg	45.27	J/molxK	100.12	Joback Method
cpg	45.27	J/molxK	100.12	Joback Method

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
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=C592176&Units=SI

Legend

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

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