

# Urea, 1,3-bis (2,2,2-trifluoroethyl)-

<b>Inchi:</b>	InChI=1S/C5H6F6N2O/c6-4(7,8)1-12-3(14)13-2-5(9,10)11/h1-2H2,(H2,12,13,14)
<b>InchiKey:</b>	NLTKGUVQZXMRSZ-UHFFFAOYSA-N
<b>Formula:</b>	C5H6F6N2O
<b>SMILES:</b>	O=C(NCC(F)(F)F)NCC(F)(F)F
<b>Mol. weight [g/mol]:</b>	224.10
<b>CAS:</b>	406-11-1

## Physical Properties

Property code	Value	Unit	Source
gf	-1122.10	kJ/mol	Joback Method
hf	-1346.33	kJ/mol	Joback Method
hfus	24.15	kJ/mol	Joback Method
hvap	38.85	kJ/mol	Joback Method
log10ws	-2.37		Crippen Method
logp	1.410		Crippen Method
mcvol	113.460	ml/mol	McGowan Method
pc	2950.48	kPa	Joback Method
tb	457.17	K	Joback Method
tc	613.53	K	Joback Method
tf	309.74	K	Joback Method
vc	0.477	m3/kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	276.09	J/molxK	457.17	Joback Method
cpg	285.48	J/molxK	483.23	Joback Method
cpg	294.29	J/molxK	509.29	Joback Method
cpg	302.56	J/molxK	535.35	Joback Method
cpg	310.30	J/molxK	561.41	Joback Method
cpg	317.54	J/molxK	587.47	Joback Method
cpg	324.30	J/molxK	613.53	Joback Method

# Sources

<b>Crippen Method:</b>	<a href="https://www.chemeo.com/doc/models/crippen_log10ws">https://www.chemeo.com/doc/models/crippen_log10ws</a>
<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=C406111&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=C406111&amp;Units=SI</a>
<b>Crippen Method:</b>	<a href="http://pubs.acs.org/doi/abs/10.1021/ci9903071">http://pubs.acs.org/doi/abs/10.1021/ci9903071</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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