

# Cycluron, HFBA

<b>Inchi:</b>	InChI=1S/C15H21F7N2O2/c1-23(2)12(26)24(10-8-6-4-3-5-7-9-10)11(25)13(16,17)14(18,
<b>InchiKey:</b>	DYNXJNPBXVDLSI-UHFFFAOYSA-N
<b>Formula:</b>	C15H21F7N2O2
<b>SMILES:</b>	CN(C)C(=O)N(C(=O)C(F)(F)C(F)(F)C(F)(F)F)C1CCCCCCC1
<b>Mol. weight [g/mol]:</b>	394.33

## Physical Properties

Property code	Value	Unit	Source
gf	-1315.76	kJ/mol	Joback Method
hf	-1800.05	kJ/mol	Joback Method
hfus	30.80	kJ/mol	Joback Method
hvap	57.73	kJ/mol	Joback Method
log10ws	-5.07		Crippen Method
logp	4.442		Crippen Method
mvol	246.840	ml/mol	McGowan Method
pc	1551.22	kPa	Joback Method
rinpol	1719.00		NIST Webbook
rinpol	1719.00		NIST Webbook
tb	688.51	K	Joback Method
tc	871.81	K	Joback Method
tf	435.34	K	Joback Method
vc	0.933	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	761.56	J/molxK	688.51	Joback Method
cpg	779.00	J/molxK	719.06	Joback Method
cpg	795.18	J/molxK	749.61	Joback Method
cpg	810.18	J/molxK	780.16	Joback Method
cpg	824.07	J/molxK	810.71	Joback Method
cpg	836.92	J/molxK	841.26	Joback Method
cpg	848.80	J/molxK	871.81	Joback Method

# Sources

<b>NIST Webbook:</b>	<a href="http://webbook.nist.gov/cgi/cbook.cgi?ID=R220270&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=R220270&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>
<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>

# 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>hvp:</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>rinp:</b>	Non-polar retention indices
<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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