

# Monolinuron, HFBA

<b>Inchi:</b>	InChI=1S/C13H10ClF7N2O3/c1-22(26-2)10(25)23(8-5-3-7(14)4-6-8)9(24)11(15,16)12(17)
<b>InchiKey:</b>	PFPSQTVOEJXIU-UHFFFAOYSA-N
<b>Formula:</b>	C13H10ClF7N2O3
<b>SMILES:</b>	CON(C)C(=O)N(C(=O)C(F)(F)C(F)(F)C(F)(F)F)c1ccc(Cl)cc1
<b>Mol. weight [g/mol]:</b>	410.67

## Physical Properties

Property code	Value	Unit	Source
gf	-1347.00	kJ/mol	Joback Method
hf	-1723.67	kJ/mol	Joback Method
hfus	37.02	kJ/mol	Joback Method
hvap	62.24	kJ/mol	Joback Method
log10ws	-4.62		Crippen Method
logp	4.119		Crippen Method
mvol	223.870	ml/mol	McGowan Method
pc	1826.28	kPa	Joback Method
rinpol	1649.00		NIST Webbook
rinpol	1649.00		NIST Webbook
tb	706.17	K	Joback Method
tc	891.81	K	Joback Method
tf	503.55	K	Joback Method
vc	0.864	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	628.66	J/mol×K	706.17	Joback Method
cpg	639.54	J/mol×K	737.11	Joback Method
cpg	649.53	J/mol×K	768.05	Joback Method
cpg	658.70	J/mol×K	798.99	Joback Method
cpg	667.12	J/mol×K	829.93	Joback Method
cpg	674.85	J/mol×K	860.87	Joback Method
cpg	681.98	J/mol×K	891.81	Joback Method

# Sources

<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=R220403&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=R220403&amp;Units=SI</a>
<b>Crippen Method:</b>	<a href="http://pubs.acs.org/doi/abs/10.1021/ci990307I">http://pubs.acs.org/doi/abs/10.1021/ci990307I</a>
<b>Crippen Method:</b>	<a href="https://www.cheméo.com/doc/models/crippen_log10ws">https://www.cheméo.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>

# 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>h vap:</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>r in pol:</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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