

# Metobromuron, HFBA

**Inchi:** InChI=1S/C13H10BrF7N2O3/c1-22(26-2)10(25)23(8-5-3-7(14)4-6-8)9(24)11(15,16)12(17)  
**InchiKey:** SKXLZQRZEZRXDM-UHFFFAOYSA-N  
**Formula:** C13H10BrF7N2O3  
**SMILES:** CON(C)C(=O)N(C(=O)C(F)(F)C(F)(F)C(F)(F)F)c1ccc(Br)cc1  
**Mol. weight [g/mol]:** 455.12

## Physical Properties

Property code	Value	Unit	Source
gf	-1320.75	kJ/mol	Joback Method
hf	-1681.60	kJ/mol	Joback Method
hfus	38.11	kJ/mol	Joback Method
hvap	64.29	kJ/mol	Joback Method
log10ws	-5.10		Crippen Method
logp	4.228		Crippen Method
mvol	229.130	ml/mol	McGowan Method
pc	2003.70	kPa	Joback Method
rinpol	1742.00		NIST Webbook
rinpol	1742.00		NIST Webbook
tb	734.90	K	Joback Method
tc	927.06	K	Joback Method
tf	533.43	K	Joback Method
vc	0.876	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	639.59	J/mol×K	734.90	Joback Method
cpg	649.89	J/mol×K	766.93	Joback Method
cpg	659.32	J/mol×K	798.95	Joback Method
cpg	667.97	J/mol×K	830.98	Joback Method
cpg	675.91	J/mol×K	863.01	Joback Method
cpg	683.24	J/mol×K	895.04	Joback Method
cpg	690.04	J/mol×K	927.06	Joback Method

# Sources

<b>NIST Webbook:</b>	<a href="http://webbook.nist.gov/cgi/cbook.cgi?ID=R220389&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=R220389&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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