

Monuron, HFBA

Inchi:	InChI=1S/C13H10ClF7N2O2/c1-22(2)10(25)23(8-5-3-7(14)4-6-8)9(24)11(15,16)12(17,18)
InchiKey:	BFXDEBCMYRXRTM-UHFFFAOYSA-N
Formula:	C13H10ClF7N2O2
SMILES:	CN(C)C(=O)N(C(=O)C(F)(F)C(F)(F)C(F)(F)F)c1ccc(Cl)cc1
Mol. weight [g/mol]:	394.67

Physical Properties

Property code	Value	Unit	Source
gf	-1242.00	kJ/mol	Joback Method
hf	-1591.45	kJ/mol	Joback Method
hfus	35.83	kJ/mol	Joback Method
hvap	59.83	kJ/mol	Joback Method
log10ws	-4.55		Crippen Method
logp	4.188		Crippen Method
mcvol	218.000	ml/mol	McGowan Method
pc	1853.11	kPa	Joback Method
rinpol	1647.00		NIST Webbook
rinpol	1647.00		NIST Webbook
tb	683.75	K	Joback Method
tc	869.63	K	Joback Method
tf	481.32	K	Joback Method
vc	0.846	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	603.50	J/molxK	683.75	Joback Method
cpg	614.74	J/molxK	714.73	Joback Method
cpg	625.04	J/molxK	745.71	Joback Method
cpg	634.48	J/molxK	776.69	Joback Method
cpg	643.14	J/molxK	807.67	Joback Method
cpg	651.12	J/molxK	838.65	Joback Method
cpg	658.49	J/molxK	869.63	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R220418&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.cheméo.com/doc/models/crippen_log10ws
Joback Method:	https://en.wikipedia.org/wiki/Joback_method

Legend

cpg:	Ideal gas heat capacity
gf:	Standard Gibbs free energy of formation
hf:	Enthalpy of formation at standard conditions
hfus:	Enthalpy of fusion at standard conditions
h vap:	Enthalpy of vaporization at standard conditions
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
pc:	Critical Pressure
r in pol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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