

(phosphonomethyl)glycine

Other names:	Glyphosate N-(phosphonomethyl)glycine
Inchi:	InChI=1S/C3H8NO5P/c5-3(6)1-4-2-10(7,8)9/h4H,1-2H2,(H,5,6)(H2,7,8,9)
InchiKey:	XDDAORKBJWWYJS-UHFFFAOYSA-N
Formula:	C3H8NO5P
SMILES:	O=C(O)C[NH2+]CP(=O)([O-])O
Mol. weight [g/mol]:	169.07

Physical Properties

Property code	Value	Unit	Source
logp	-2.862		Crippen Method
mcvol	108.620	ml/mol	McGowan Method
tf	487.80	K	Solid-liquid phase equilibrium of glyphosate in selected solvents

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Cheméo Relay (1.0):	
Cheméo Relay (1.0, beta):	
Solid-liquid phase equilibrium of glyphosate in selected solvents:	https://www.doi.org/10.1016/j.fluid.2012.05.003
Solubility of Glyphosate in Ethanol + Water, 1-Propanol + Water, and 2-Propanol + Water from (293 to 333) K:	https://www.doi.org/10.1021/je901006c

Legend

logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
tf:	Normal melting (fusion) point

Latest version available from:

<https://www.chemeo.com/cid/112-507-4/phosphonomethyl-glycine.pdf>

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