

9H-Carbazole, 3,6-dinitro-

Other names:	3,6-Dinitrocarbazole 3,6-dinitro-9H-carbazole Carbazole, 3,6-dinitro-
Inchi:	InChI=1S/C12H7N3O4/c16-14(17)7-1-3-11-9(5-7)10-6-8(15(18)19)2-4-12(10)13-11/h1-6
InchiKey:	IARXLBTXILYASE-UHFFFAOYSA-N
Formula:	C12H7N3O4
SMILES:	O=[N+](O-)c1ccc2[nH]c3ccc([N+](=O)[O-])cc3c2c1
Mol. weight [g/mol]:	257.20
CAS:	3244-54-0

Physical Properties

Property code	Value	Unit	Source
log10ws	-5.60		Crippen Method
logp	2.656		Crippen Method
mcvol	166.380	ml/mol	McGowan Method
tf	569.65	K	On the melting temperatures of 3,6-diamino-9H-carbazole and 3,6-dinitro-9H-carbazole

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
On the melting temperatures of 3,6-diamino-9H-carbazole and 3,6-dinitro-9H-carbazole:	https://www.doi.org/10.1016/j.tca.2005.05.013
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C3244540&Units=SI

Legend

log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient

mcvol: McGowan's characteristic volume

tf: Normal melting (fusion) point

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