1,3,5-Triazine-2,4-diamine, N,N'-diethyl-6-methoxy-

Other names:	s-Triazine, 2,4-bis(ethylamino)-6-methoxy-
	G-30044
	Geigy 30,044
	Gesadural
	Pimeton
	Simeton
	Simetone
	Methoxy simazine
	2-Methoxy-4,6-bis(ethylamino)-s-triazine
	2,4-Bis(ethylamino)-6-methoxy-s-triazine
	4,6-Bis(ethylamino)-2-methoxy-s-triazine
	2-Methoxy-4,6-bis(ethylamino)-1,3,5-triazine
	NSC 163050
	N,N'-diethyl-6-methoxy-1,3,5-triazine-2,4-diamine
Inchi:	InChI=1S/C8H15N5O/c1-4-9-6-11-7(10-5-2)13-8(12-6)14-3/h4-5H2,1-3H3,(H2,9,10,11,12
InchiKey:	HKAMKLBXTLTVCN-UHFFFAOYSA-N
Formula:	C8H15N5O
SMILES:	CCNc1nc(NCC)nc(OC)n1
Mol. weight [g/mol]:	197.24
CAS:	673-04-1

Physical Properties

Property code	Value	Unit	Source
log10ws	-1.74		Crippen Method
logp	0.744		Crippen Method
mcvol	155.590	ml/mol	McGowan Method
ripol	2680.00		NIST Webbook
ripol	2714.00		NIST Webbook
ripol	2680.00		NIST Webbook

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
hsubt	98.20	kJ/mol	363.00	NIST Webbook

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C673041&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

Legend

hsubt:	Enthalpy of sublimation at a given temperature
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
ripol:	Polar retention indices

Latest version available from:

https://www.chemeo.com/cid/36-451-1/1-3-5-Triazine-2-4-diamine-N-N-diethyl-6-methoxy.pdf

Generated by Cheméo on 2024-10-12 09:36:03.790961897 +0000 UTC m=+3306626.427931150.

Cheméo (https://www.chemeo.com) is the biggest free database of chemical and physical data for the process industry.