

Secbumeton

Other names:	1,3,5-Triazine-2,4-diamine, N-ethyl-6-methoxy-N'-(1-methylpropyl)-s-Triazine, 2-(sec-butylamino)-4-(ethylamino)-6-methoxy-Etazin Etazine Ezitan Geigy G.S. 14254 GS 14254 Sumitol Sumitol 80W sec-Bumetone 1,3,5-Triazine-2,4-diamine, N2-ethyl-6-methoxy-N4-(1-methylpropyl)-
Inchi:	InChI=1S/C10H19N5O/c1-5-7(3)12-9-13-8(11-6-2)14-10(15-9)16-4/h7H,5-6H2,1-4H3,(H2
InchiKey:	ZJMZZNVGNSWOOM-UHFFFAOYSA-N
Formula:	C10H19N5O
SMILES:	CCNc1nc(NC(C)CC)nc(OC)n1
Mol. weight [g/mol]:	225.29
CAS:	26259-45-0

Physical Properties

Property code	Value	Unit	Source
log10ws	-2.69		Crippen Method
logp	1.522		Crippen Method
mcvol	183.770	ml/mol	McGowan Method
rinpol	1777.00		NIST Webbook
rinpol	1828.00		NIST Webbook
rinpol	1777.00		NIST Webbook
ripol	2676.00		NIST Webbook
ripol	2676.00		NIST Webbook
ripol	2676.00		NIST Webbook
ripol	2676.00		NIST Webbook
ripol	2708.00		NIST Webbook

Sources

Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C26259450&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

Legend

log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
rinpol:	Non-polar retention indices
ripol:	Polar retention indices

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