

Albendazole

Inchi:	InChI=1S/C12H15N3O2S/c1-3-6-18-8-4-5-9-10(7-8)14-11(13-9)15-12(16)17-2/h4-5,7H,3
InchiKey:	HXHWSAZORRCQMX-UHFFFAOYSA-N
Formula:	C12H15N3O2S
SMILES:	CCCS1CCC2NC(=O)OC([nH])C2C1
Mol. weight [g/mol]:	265.34
CAS:	54965-21-8

Physical Properties

Property code	Value	Unit	Source
log10ws	-5.02		Cheméo Relay (1.0)
logp	2.761		Crippen Method
mcvol	194.750	ml/mol	McGowan Method
tf	482.15	K	Jean-Claude Bradley Open Melting Point Dataset (2014, CC0)

Sources

Cheméo Relay (1.0, beta):

Jean-Claude Bradley Open Melting
Point Dataset (2014, CC0):
McGowan Method:

https://figshare.com/articles/Jean_Claude_Bradley_Open_Melting_Point_Dataset/1031637

<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):

Legend

log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
tf:	Normal melting (fusion) point

Latest version available from:

<https://www.chemeo.com/cid/104-614-4/Albendazole.pdf>

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