fenbendazole

Other names:	methyl (6-(phenylthio)-1H-benzo[d]imidazol-2-yl)carbamate
Inchi:	InChI=1S/C15H13N3O2S/c1-20-15(19)18-14-16-12-8-7-11(9-13(12)17-14)21-10-5-3-2-4-
InchiKey:	HDDSHPAODJUKPD-UHFFFAOYSA-N
Formula:	C15H13N3O2S
SMILES:	COC(=O)Nc1nc2ccc(Sc3ccccc3)cc2[nH]1
Mol. weight [g/mol]:	299.35

Physical Properties

Property code	Value	Unit	Source
log10ws	-5.69		Cheméo Relay (1.0)
logp	3.411		Crippen Method
mcvol	213.260	ml/mol	McGowan Method
tf	527.64	K	Cheméo Relay (1.0)

Sources

Cheméo Relay (1.0):	
Cheméo Relay (1.0, beta):	
Equilibrium Solubility Determination and Modeling of Fenbendazole in Cosolvent Mixtures at (283.15-328.15) K:	https://www.doi.org/10.1021/acs.jced.9b00471
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

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/102-266-3/fenbendazole.pdf

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