Heptabarbital, 1,3-dibutyl

Other names:	Heptabarbital perbutylated
	Heptobarbital butylated
Inchi:	InChI=1S/C21H34N2O3/c1-4-7-15-22-18(24)21(6-3,17-13-11-9-10-12-14-17)19(25)23(20
InchiKey:	MDUSDFNVLVIWCQ-UHFFFAOYSA-N
Formula:	C21H34N2O3
SMILES:	CCCCN1C(=O)N(CCCC)C(=O)C(CC)(C2=CCCCCC2)C1=O
Mol. weight [g/mol]:	362.51

Physical Properties

Property code	Value	Unit	Source
log10ws	-5.46		Crippen Method
logp	4.664		Crippen Method
mcvol	305.400	ml/mol	McGowan Method
rinpol	2343.00		NIST Webbook

Sources

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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R387898&Units=SI

Legend

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