ETAMIPHYLLINE

Other names: 1H-Purine-2,6-dione, 7-[2-(diethylamino)ethyl]-3,7-dihydro-1,3-dimethyl-
Camphophyline
Corafil
Diaethylaminoaethyl-theophyllin
Diethylaminoethyltheophylline
Etaminophylline
Etamiphylline
Milliphylline
Millophyline
Parephyllin
Queryl
R-3588
Solufilina
Soluphyline
Theophylline, 7-(2-(diethylamino)ethyl)-
1,3-Dimethyl-7-(2-(diethylamino)ethyl)xanthine
7-(2-(Diethylamino)ethyl)-1,3-dimethylxanthine
7-(2-(Diethylamino)ethyl)theophylline
Millophylline
Dietamiphylline
7-[2-(Diethylamino)ethyl]-3,7-dihydro-1,3-dimethyl-1H-purine-2,6-dione
7-(Diethylaminoethyl)theophylline
NSC 38348

Inchi: InChI=1S/C13H21N5O2/c1-5-17(6-2)7-8-18-9-14-11-10(18)12(19)16(4)13(20)15(11)3/h9

InchiKey: AWKLBIOQCIORSB-UHFFFAOYSA-N

Formula: C13H21N5O2

SMILES: CCN(CC)CCn1cnc2c1c(=O)n(C)c(=O)n2C

Mol. weight [g/mol]: 279.34

Physical Properties

Property code	Value	Unit	Source
ie	7.95	eV	Cheméo Relay (1.0)
log10ws	-0.58		Cheméo Relay (1.0)
logp	-0.225		Crippen Method
mcvol	216.750	ml/mol	McGowan Method
tf	398.42	K	Cheméo Relay (1.0)

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C314352&Units=SI
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
Cheméo Relay (1.0):	
Cheméo Relay (1.0, beta):	

Legend

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