CYCLOTHIAZIDE

Other names:

2H-1,2,4-Benzothiadiazine-7-sulfonamide, 3-bicyclo[2.2.1]hept-5-en-2-yl-6-chloro-3,4-dihydro-, 1,1-dioxide
2H-1,2,4-Benzothiadiazine-7-sulfonamide, 3,4-dihydro-6-chloro-3-(5-norbornen-2-yl)-,1,1-dioxide
Annhydron
Aquirel
Doburil
MDi 193
Renazide
Valmiran

6-Chloro-3,4-dihydro-3-(5-norbornen-2-yl)-2H-1,2,4-benzothiadiazine-7-sulfonamide 1,1-dioxide
Fluid
Lilly 35483
2H-1,2,4-Benzothiadiazine-7-sulfonamide, 6-chloro-3,4-dihydro-3-(5-norbornen-2-yl)-, 1,1-dioxide

Inchi: InChI=1S/C14H16ClN3O4S2/c15-10-5-11-13(6-12(10)23(16,19)20)24(21,22)18-14(17-11

InchiKey: BOCUKUHCLICSIY-UHFFFAOYSA-N

Formula: C14H16ClN3O4S2

SMILES: NS(=O)(=O)c1cc2c(cc1Cl)NC(C1CC3C=CC1C3)NS2(=O)=O

Mol. weight [g/mol]: 389.89

Physical Properties

Property code	Value	Unit	Source
hfus	68.25	kJ/mol	Joback Method
log10ws	-4.07		Cheméo Relay (1.0)
logp	1.230		Crippen Method
mcvol	245.840	ml/mol	McGowan Method
tf	540.85	K	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	738.32	J/mol×K	866.26	Joback Method
cpg	751.70	J/mol×K	906.99	Joback Method
cpg	763.64	J/mol×K	947.71	Joback Method
cpg	774.21	J/mol×K	988.44	Joback Method
cpg	783.48	J/mol×K	1029.16	Joback Method

cpg	791.53	J/mol×K	1069.89	Joback Method
cpg	798.43	J/mol×K	1110.62	Joback Method

Sources

Cheméo Relay (1.0, beta):

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C2259963&Units=SI

Joback Method: https://en.wikipedia.org/wiki/Joback_method

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):

Legend

cpg: Ideal gas heat capacity

hfus: Enthalpy of fusion at standard conditions

log10ws: Log10 of Water solubility in mol/l

logp: Octanol/Water partition coefficient

mcvol: McGowan's characteristic volume

tf: Normal melting (fusion) point