2,4,6(1H,3H,5H)-Pyrimidinetrione, 5-(1-cyclohepten-1-yl)-5-ethyl-

Other names: 5-(1-Cyclohepten-1-Yl)-5-ethyl-2,4,6(1H,3H,5H)-pyrimidinetrione
5-(1-Cyclohepten-1-yl)-5-ethylbarbituric acid
5-(1-cycloheptenyl)-5-ethyl-1,3-diazinane-2,4,6-trione
5-(Cyclohepten-1-yl)-5-ethylbarbituric acid
5-Ethyl-5-(1'-cycloheptenyl)-barbituric acid
5-Ethyl-5-cycloheptenylbarbituric acid
Barbituric acid, 5-(1-cyclohepten-1-yl)-5-ethyl-
Cycloheptenylethylbarbituric acid
Cycloheptenylethylmalonylurea
G 475
Heptabarb
Heptabarbitone
Heptabarbum
Heptadorm
Heptamal
Heptbarbital
Medapan
Medomin
Medomine
Noctyn

Inchi: InChI=1S/C13H18N2O3/c1-2-13(9-7-5-3-4-6-8-9)10(16)14-12(18)15-11(13)17/h7H,2-6,8

InchiKey: PAZQYDJGLKSCSI-UHFFFAOYSA-N

Formula: C13H18N2O3

SMILES: CCC1(C2=CCCCCC2)C(=O)NC(=O)NC1=O

Mol. weight [g/mol]: 250.30

Physical Properties

Property code	Value	Unit	Source
hfus	22.17	kJ/mol	Joback Method
log10ws	-3.00		Aqueous Solubility Prediction Method
logp	1.639		Crippen Method
mcvol	192.680	ml/mol	McGowan Method
rinpol	2032.00		NIST Webbook
rinpol	2036.00		NIST Webbook
rinpol	2098.00		NIST Webbook
rinpol	2035.00		NIST Webbook

rinpol	2045.00		NIST Webbook
rinpol	2070.00		NIST Webbook
rinpol	2047.00		NIST Webbook
rinpol	2041.00		NIST Webbook
rinpol	2032.00		NIST Webbook
rinpol	2032.00		NIST Webbook
rinpol	2065.00		NIST Webbook
rinpol	2036.00		NIST Webbook
rinpol	2090.00		NIST Webbook
rinpol	2075.00		NIST Webbook
rinpol	2067.00		NIST Webbook
rinpol	2067.00		NIST Webbook
rinpol	2098.00		NIST Webbook
rinpol	2058.00		NIST Webbook
rinpol	2098.00		NIST Webbook
rinpol	2070.00		NIST Webbook
tf	447.35	K	Aqueous Solubility Prediction Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	629.40	J/mol×K	849.82	Joback Method
cpg	649.78	J/mol×K	897.44	Joback Method
cpg	668.51	J/mol×K	945.07	Joback Method
cpg	685.62	J/mol×K	992.69	Joback Method
cpg	701.12	J/mol×K	1040.31	Joback Method
cpg	715.03	J/mol×K	1087.94	Joback Method
cpg	727.38	J/mol×K	1135.56	Joback Method

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C509864&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

Cheméo Relay (1.0):

Cheméo Relay (1.0, beta):

Aqueous Solubility Prediction Method: http://onschallenge.wikispaces.com/file/view/AqueousDataset002.xlsx/351826032/AqueousDa

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
rinpol:	Non-polar retention indices
tf:	Normal melting (fusion) point