Thialbarbital

Other names: 4,6(1H,5H)-Pyrimidinedione, 5-(2-cyclohexen-1-yl)dihydro-5-(2-propenyl)-2-thioxo-
Barbituric acid, 5-allyl-5-(2-cyclohexen-1-yl)-2-thio-
5-Allyl-5-(2-cyclohexen-1-yl)-2-thiobarbituric acid
5-«delta»(2:3)-Cyclohexenyl-5-allyl-2-thiobarbituric acid
Kemithal
Thialbarbitone
Thialpenton
Thiohexallymalum
5-Allyl-5-(2-cyclohexen-1-yl)-2-thioxodihydro-4,6(1H,5H)-pyrimidinedione

Inchi: InChI=1S/C13H16N2O2S/c1-2-8-13(9-6-4-3-5-7-9)10(16)14-12(18)15-11(13)17/h2,4,6,9H

InchiKey: PXLVRFQEBVNJOH-UHFFFAOYSA-N

Formula: C13H16N2O2S

SMILES: C=CCC1(C2C=CCCC2)C(=O)NC(=S)NC1=O

Mol. weight [g/mol]: 264.34

CAS: 467-36-7

Physical Properties

Property code	Value	Unit	Source
gf	240.88	kJ/mol	Joback Method
hf	-89.24	kJ/mol	Joback Method
hfus	30.97	kJ/mol	Joback Method
hvap	73.35	kJ/mol	Joback Method
log10ws	-3.55		Crippen Method
logp	1.436		Crippen Method
mcvol	198.860	ml/mol	McGowan Method
pc	3269.04	kPa	Joback Method
rinpol	2116.00		NIST Webbook
rinpol	2116.00		NIST Webbook
tb	837.40	K	Joback Method
tc	1123.73	K	Joback Method
tf	684.10	K	Joback Method
vc	0.721	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	599.47	J/mol×K	837.40	Joback Method
cpg	618.35	J/mol×K	885.12	Joback Method
cpg	636.27	J/mol×K	932.84	Joback Method
cpg	653.38	J/mol×K	980.57	Joback Method
cpg	669.84	J/mol×K	1028.29	Joback Method
cpg	685.83	J/mol×K	1076.01	Joback Method
cpg	701.50	J/mol×K	1123.73	Joback Method

Sources

Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws
Joback Method: https://en.wikipedia.org/wiki/Joback_method
McGowan Method: http://link.springer.com/article/10.1007/BF02311772
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C467367&Units=SI

Legend

cpg: Ideal gas heat capacity
gf: Standard Gibbs free energy of formation
hf: Enthalpy of formation at standard conditions
hfus: Enthalpy of fusion at standard conditions
hvap: Enthalpy of vaporization at standard conditions
log10ws: Log10 of Water solubility in mol/l
logp: Octanol/Water partition coefficient
mcvol: McGowan's characteristic volume
pc: Critical Pressure
rinpol: Non-polar retention indices
tb: Normal Boiling Point Temperature
tc: Critical Temperature
tf: Normal melting (fusion) point
vc: Critical Volume