Methallatal

Other names:	5-Ethyl-5-(2-methylallyl)-2-thiobarbituric acid 4,6(1H,5H)-Pyrimidinedione, 5-ethyldihydro-5-(2-methyl-2-propenyl)-2-thioxo- Barbituric acid, 5-ethyl-5-(2-methylallyl)-2-thio- Mosidal V 12 5-Ethyldihydro-5-(2-methyl-2-propenyl)-2-thioxo-4,6(1H,5H)-pyrimidinedione 5-Ethyl-5-(2-methyl-2-propenyl)-2-thioxodihydro-4,6(1H,5H)-pyrimidinedione 5-ethyldihydro-5-(2-methylallyl)-2-thioxo-1H,5H-pyrimidine-4,6-dione
Inchi:	InChI=1S/C10H14N2O2S/c1-4-10(5-6(2)3)7(13)11-9(15)12-8(10)14/h2,4-5H2,1,3H3,(H2
InchiKey:	XMQICEWOKPEQRG-UHFFFAOYSA-N
Formula:	C10H14N2O2S
SMILES:	C=C(C)CC1(CC)C(=O)NC(=S)NC1=O
Mol. weight [g/mol]:	226.29
CAS:	115-56-0

Physical Properties

Property code	Value	Unit	Source
gf	152.66	kJ/mol	Joback Method
hf	-149.21	kJ/mol	Joback Method
hfus	28.84	kJ/mol	Joback Method
hvap	66.03	kJ/mol	Joback Method
log10ws	-2.79		Crippen Method
logp	0.880		Crippen Method
mcvol	171.750	ml/mol	McGowan Method
pc	3472.45	kPa	Joback Method
rinpol	1736.00		NIST Webbook
tb	749.93	K	Joback Method
tc	1015.84	K	Joback Method
tf	628.19	K	Joback Method
vc	0.634	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source

cpg	468.10	J/mol×K	749.93	Joback Method
cpg	484.05	J/mol×K	794.25	Joback Method
cpg	499.36	J/mol×K	838.57	Joback Method
cpg	514.13	J/mol×K	882.88	Joback Method
cpg	528.46	J/mol×K	927.20	Joback Method
cpg	542.46	J/mol×K	971.52	Joback Method
cpg	556.23	J/mol×K	1015.84	Joback Method

Sources

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=C115560&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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

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