Propallylonal

Other names: 2,4,6(1H,3H,5H)-Pyrimidinetrione, 5-(2-bromo-2-propenyl)-5-(1-methylethyl)-
Barbituric acid, 5-(2-bromoallyl)-5-isopropyl-
5-(2'-Bromallyl)-5-isopropylbarbituric acid
Bromoaprobarbital
5-(2-Bromo-2-propenyl)-5-(1-methylethyl)-2,4,6(1H,3H,5H)-pyrimidinetrione
Ibomal
5-Isopropyl-5-bromallylbarbituric acid
5-Isopropyl-5-(2-bromoallyl)barbituate
Kwietal
Noctal
Noctenal
Nostal
Nostral
Propaldon
Quietal
Quietalum
5-(2-Bromoallyl)-5-isopropylbarbituric acid
5-Isopropyl-5-bromoallylbarbituric acid
5-Isopropyl-5-(2-bromoallyl)barbiturate
5-(«beta»-Bromoallyl)-5-isopropylbarbituric acid

Inchi: InChI=1S/C10H13BrN2O3/c1-5(2)10(4-6(3)11)7(14)12-9(16)13-8(10)15/h5H,3-4H2,1-2H

InchiKey: KTGWBBOJAGDSHN-UHFFFAOYSA-N

Formula: C10H13BrN2O3

SMILES: C=C(Br)CC1(C(C)C)C(=O)NC(=O)NC1=O

Mol. weight [g/mol]: 289.13

CAS: 545-93-7

Physical Properties

Property code	Value	Unit	Source
gf	-48.90	kJ/mol	Joback Method
hf	-380.96	kJ/mol	Joback Method
hfus	24.07	kJ/mol	Joback Method
hvap	68.85	kJ/mol	Joback Method
log10ws	-2.88		Crippen Method
logp	1.293		Crippen Method
mcvol	178.770	ml/mol	McGowan Method
pc	3677.55	kPa	Joback Method

rinpol	1890.00		NIST Webbook
rinpol	1866.00		NIST Webbook
rinpol	1875.00		NIST Webbook
rinpol	1883.00		NIST Webbook
rinpol	1875.00		NIST Webbook
rinpol	1883.00		NIST Webbook
rinpol	1866.00		NIST Webbook
tb	810.83	K	Joback Method
tc	1087.84	K	Joback Method
tf	677.54	K	Joback Method
vc	0.659	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	506.29	J/mol×K	810.83	Joback Method
cpg	522.82	J/mol×K	857.00	Joback Method
cpg	538.42	J/mol×K	903.17	Joback Method
cpg	553.14	J/mol×K	949.34	Joback Method
cpg	567.00	J/mol×K	995.50	Joback Method
cpg	580.04	J/mol×K	1041.67	Joback Method
cpg	592.31	J/mol×K	1087.84	Joback Method

Sources

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=C545937&Units=SI
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws

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