Brallobarbital

Other names:	2,4,6(1H,3H,5H)-Pyrimidinetrione, 5-(2-bromo-2-propenyl)-5-(2-propenyl)-
	Barbituric acid, 5-allyl-5-(2-bromoallyl)-
	Allylbromoallylbarbituric acid
	U. C. B. 5033
	Ucedorm
	Vesperone
	5-(2'-Bromallyl)-5-allylbarbituric acid
	5-Allyl-5-(2-bromoallyl)barbituric acid
	Brallobarbitone
	5-Allyl-5-(2-bromoallyl)-2,4,6(1H,3H,5H)-pyrimidinetrione
	2,4,6(1H,3H,5H)-Pyrimidinetrione, 5-(2-bromo-2-propen-1-yl)-5-(2-propen-1-yl)-
Inchi:	InChI=1S/C10H11BrN2O3/c1-3-4-10(5-6(2)11)7(14)12-9(16)13-8(10)15/h3H,1-2,4-5H2,(
InchiKey:	DYODAJAEQDVYFX-UHFFFAOYSA-N
Formula:	C10H11BrN2O3
SMILES:	C=CCC1(CC(=C)Br)C(=O)NC(=O)NC1=O
Mol. weight [g/mol]:	287.11
CAS:	561-86-4

Physical Properties

Property code	Value	Unit	Source
gf	41.38	kJ/mol	Joback Method
hf	-250.25	kJ/mol	Joback Method
hfus	26.32	kJ/mol	Joback Method
hvap	68.56	kJ/mol	Joback Method
log10ws	-2.98		Crippen Method
logp	1.214		Crippen Method
mcvol	174.470	ml/mol	McGowan Method
pc	3834.03	kPa	Joback Method
rinpol	1842.00		NIST Webbook
rinpol	1858.00		NIST Webbook
rinpol	1828.00		NIST Webbook
rinpol	1828.00		NIST Webbook
rinpol	1850.00		NIST Webbook
rinpol	1865.00		NIST Webbook
rinpol	1842.00		NIST Webbook
tb	807.95	K	Joback Method
tc	1085.15	K	Joback Method

tf	690.78	K	Joback Method
vc	0.646	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	479.54	J/mol×K	807.95	Joback Method
cpg	495.15	J/mol×K	854.15	Joback Method
cpg	509.93	J/mol×K	900.35	Joback Method
cpg	523.94	J/mol×K	946.55	Joback Method
cpg	537.23	J/mol×K	992.75	Joback Method
cpg	549.84	J/mol×K	1038.95	Joback Method
cpg	561.83	J/mol×K	1085.15	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=C561864&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

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