

Barbituric acid, 5-(2-bromoallyl)-5-propyl-

Other names:	5-(2-Bromoallyl)-5-propylbarbituric acid 5-(n-Propyl)-5-(2-bromoallyl)barbituric acid 5-(2-Bromo-2-propenyl)-5-propyl-hexahydropyrimidin-2,4,6-trione Brallobarbital, dihydro- Brallobarbital M (dihydro)
Inchi:	InChI=1S/C10H13BrN2O3/c1-3-4-10(5-6(2)11)7(14)12-9(16)13-8(10)15/h2-5H2,1H3,(H2
InchiKey:	ISWRUGBQYRDOGS-UHFFFAOYSA-N
Formula:	C10H13BrN2O3
SMILES:	C=C(Br)CC1(CCC)C(=O)NC(=O)NC1=O
Mol. weight [g/mol]:	289.13
CAS:	91062-54-3

Physical Properties

Property code	Value	Unit	Source
gf	-46.46	kJ/mol	Joback Method
hf	-375.68	kJ/mol	Joback Method
hfus	27.60	kJ/mol	Joback Method
hvap	69.23	kJ/mol	Joback Method
log10ws	-3.12		Crippen Method
logp	1.438		Crippen Method
mcvol	178.770	ml/mol	McGowan Method
pc	3642.13	kPa	Joback Method
rinpol	1970.00		NIST Webbook
tb	811.27	K	Joback Method
tc	1082.84	K	Joback Method
tf	692.54	K	Joback Method
vc	0.665	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	505.71	J/mol×K	811.27	Joback Method
cpg	521.93	J/mol×K	856.53	Joback Method
cpg	537.28	J/mol×K	901.79	Joback Method

cpg	551.80	J/mol×K	947.05	Joback Method
cpg	565.51	J/mol×K	992.32	Joback Method
cpg	578.46	J/mol×K	1037.58	Joback Method
cpg	590.68	J/mol×K	1082.84	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=C91062543&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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