Brallobarbital M (OH)

Inchi: InChI=1S/C10H13BrN2O4/c1-5(11)3-10(4-6(2)14)7(15)12-9(17)13-8(10)16/h6,14H,1,3-4
InchiKey: HXQWYZCJEPDVCB-UHFFFAOYSA-N
Formula: C10H13BrN2O4
SMILES: C=C(Br)CC1(CC(C)O)C(=O)NC(=O)NC1=O
Mol. weight [g/mol]: 305.12

Physical Properties

Property code	Value	Unit	Source
gf	-185.72	kJ/mol	Joback Method
hf	-533.19	kJ/mol	Joback Method
hfus	28.16	kJ/mol	Joback Method
hvap	85.52	kJ/mol	Joback Method
log10ws	-2.50		Crippen Method
logp	0.408		Crippen Method
mcvol	184.640	ml/mol	McGowan Method
pc	4124.99	kPa	Joback Method
rinpol	2040.00		NIST Webbook
tb	903.01	K	Joback Method
tc	1155.76	K	Joback Method
tf	738.36	K	Joback Method
vc	0.678	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	556.77	J/mol×K	903.01	Joback Method
cpg	570.36	J/mol×K	945.14	Joback Method
cpg	583.22	J/mol×K	987.26	Joback Method
cpg	595.39	J/mol×K	1029.39	Joback Method
cpg	606.91	J/mol×K	1071.51	Joback Method
cpg	617.81	J/mol×K	1113.64	Joback Method
cpg	628.11	J/mol×K	1155.76	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=R57309&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