5-(3-Methyl-2-butenyl)-5-isoPrbarbital

Inchi: InChI=1S/C12H18N2O3/c1-7(2)5-6-12(8(3)4)9(15)13-11(17)14-10(12)16/h5,8H,6H2,1-4H
InchiKey: ZCDHRBAYNFWZBH-UHFFFAOYSA-N
Formula: C12H18N2O3
SMILES: CC(C)=CCC1(C(C)C)C(=O)NC(=O)NC1=O
Mol. weight [g/mol]: 238.29

Physical Properties

Property code	Value	Unit	Source
gf	-54.00	kJ/mol	Joback Method
hf	-456.78	kJ/mol	Joback Method
hfus	25.45	kJ/mol	Joback Method
hvap	67.49	kJ/mol	Joback Method
log10ws	-2.59		Estimated Solubility Method
log10ws	-2.59		Aqueous Solubility Prediction Method
logp	1.351		Crippen Method
mcvol	189.450	ml/mol	McGowan Method
pc	2770.08	kPa	Joback Method
tb	797.91	K	Joback Method
tc	1058.37	K	Joback Method
tf	636.96	K	Joback Method
vc	0.709	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	580.79	J/mol×K	797.91	Joback Method
cpg	599.67	J/mol×K	841.32	Joback Method
cpg	617.53	J/mol×K	884.73	Joback Method
cpg	634.41	J/mol×K	928.14	Joback Method
cpg	650.37	J/mol×K	971.55	Joback Method
cpg	665.43	J/mol×K	1014.96	Joback Method
cpg	679.65	J/mol×K	1058.37	Joback Method

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
Aqueous Solubility Prediction Method:	http://onschallenge.wikispaces.com/file/view/AqueousDataset002.xlsx/351826032/AqueousDa
Estimated Solubility Method:	http://pubs.acs.org/doi/suppl/10.1021/ci034243x/suppl_file/ci034243xsi20040112_053635.txt
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume