Barbituric acid, 5-bicyclo(3.2.1)oct-2-en-3-yl-5-ethyl-

Other names: Reposal
Inchi: InChI=1S/C14H18N2O3/c1-2-14(11(17)15-13(19)16-12(14)18)10-6-8-3-4-9(5-8)7-10/h6,8
InchiKey: MKELYWOVSPVORM-UHFFFAOYSA-N
Formula: C14H18N2O3
SMILES: CCC1(C2=CC3CCC(C2)C3)C(=O)NC(=O)NC1=O
Mol. weight [g/mol]: 262.30
CAS: 3625-25-0

Physical Properties

Property code	Value	Unit	Source
gf	11.24	kJ/mol	Joback Method
hf	-420.62	kJ/mol	Joback Method
hfus	28.17	kJ/mol	Joback Method
hvap	73.42	kJ/mol	Joback Method
log10ws	-3.18		Crippen Method
logp	1.495		Crippen Method
mcvol	195.910	ml/mol	McGowan Method
pc	2999.15	kPa	Joback Method
rinpol	2092.00		NIST Webbook
rinpol	2092.00		NIST Webbook
tb	866.23	K	Joback Method
tc	1146.26	K	Joback Method
tf	735.66	K	Joback Method
vc	0.730	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	667.03	J/mol×K	866.23	Joback Method
cpg	687.51	J/mol×K	912.90	Joback Method
cpg	706.77	J/mol×K	959.57	Joback Method
cpg	724.90	J/mol×K	1006.25	Joback Method
cpg	742.00	J/mol×K	1052.92	Joback Method
cpg	758.20	J/mol×K	1099.59	Joback Method

cpg	773.60	J/mol×K	1146.26	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C3625250&Units=SI
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

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