5-Ethyl-5-(3-oxy-1-cyclohexenyl)-hexahydropyrim

Other names:	3'-Oxocyclobarbital
	Cyclobarbital, (3-oxo)-
	Barbituric acid, 5-ethyl-5-(3-oxo-1-cyclohexen-1-yl)-
	Cyclobarbital M (oxo)
Inchi:	InChI=1S/C12H14N2O4/c1-2-12(7-4-3-5-8(15)6-7)9(16)13-11(18)14-10(12)17/h6H,2-5H2
InchiKey:	QECKKEAIYXGFLF-UHFFFAOYSA-N
Formula:	C12H14N2O4
SMILES:	CCC1(C2=CC(=O)CCC2)C(=O)NC(=O)NC1=O
Mol. weight [g/mol]:	250.25
CAS:	35305-10-3

Physical Properties

Property code	Value	Unit	Source
gf	-193.33	kJ/mol	Joback Method
hf	-575.66	kJ/mol	Joback Method
hfus	21.19	kJ/mol	Joback Method
hvap	73.78	kJ/mol	Joback Method
log10ws	-2.21		Crippen Method
logp	0.428		Crippen Method
mcvol	180.160	ml/mol	McGowan Method
pc	3581.35	kPa	Joback Method
tb	890.49	K	Joback Method
tc	1183.07	K	Joback Method
tf	764.12	K	Joback Method
vc	0.660	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	596.20	J/mol×K	890.49	Joback Method
cpg	614.08	J/mol×K	939.25	Joback Method
cpg	630.18	J/mol×K	988.02	Joback Method
cpg	644.45	J/mol×K	1036.78	Joback Method
cpg	656.86	J/mol×K	1085.54	Joback Method

cpg	667.35	J/mol×K	1134.30	Joback Method
cpg	675.88	J/mol×K	1183.07	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=C35305103&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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume