Hexethal

Other names:	2,4,6(1H,3H,5H)-Pyrimidinetrione, 5-ethyl-5-hexyl-
	Barbituric acid, 5-ethyl-5-hexyl-
	Ortal
	Ortol
	5-Ethyl-5-hexylbarbituric acid
	Acide hexylethylbarbiturique
	Barbituric acid, 5-ethyl-5-n-hexyl-
	5-Ethyl-5-hexyl-2,4,6(1H,3H,5H)-pyrimidinetrione
	NSC 32303
Inchi:	InChI=1S/C12H20N2O3/c1-3-5-6-7-8-12(4-2)9(15)13-11(17)14-10(12)16/h3-8H2,1-2H3,(
InchiKey:	PSTVHRSUNBSVIJ-UHFFFAOYSA-N
Formula:	C12H20N2O3
SMILES:	CCCCCCC1(CC)C(=O)NC(=O)NC1=O
Mol. weight [g/mol]:	240.30
CAS:	77-30-5

Physical Properties

Property code	Value	Unit	Source
gf	-123.23	kJ/mol	Joback Method
hf	-558.93	kJ/mol	Joback Method
hfus	30.08	kJ/mol	Joback Method
hvap	67.84	kJ/mol	Joback Method
log10ws	-3.18		Crippen Method
logp	1.719		Crippen Method
mcvol	193.750	ml/mol	McGowan Method
pc	2589.85	kPa	Joback Method
rinpol	1858.00		NIST Webbook
rinpol	1835.00		NIST Webbook
rinpol	1835.00		NIST Webbook
tb	794.31	K	Joback Method
tc	1037.02	K	Joback Method
tf	671.00	K	Joback Method
vc	0.734	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	606.15	J/mol×K	794.31	Joback Method
cpg	624.76	J/mol×K	834.76	Joback Method
cpg	642.39	J/mol×K	875.21	Joback Method
cpg	659.04	J/mol×K	915.66	Joback Method
cpg	674.72	J/mol×K	956.12	Joback Method
cpg	689.45	J/mol×K	996.57	Joback Method
cpg	703.24	J/mol×K	1037.02	Joback Method

Sources

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=C77305&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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