5-Ethyl-5-p-tolylbarbituric acid

Other names: 2,4,6(1H,3H,5H)-Pyrimidinetrione, 5-ethyl-5-(4-methylphenyl)-
Barbituric acid, 5-ethyl-5-p-tolyl
5-ethyl-5,4'-tolylbarbituric acid
Inchi: InChI=1S/C13H14N2O3/c1-3-13(9-6-4-8(2)5-7-9)10(16)14-12(18)15-11(13)17/h4-7H,3H2
InchiKey: ZYJDWGKPBQDCBX-UHFFFAOYSA-N
Formula: C13H14N2O3
SMILES: CCC1(c2ccc(C)cc2)C(=O)NC(=O)NC1=O
Mol. weight [g/mol]: 246.26
CAS: 52584-39-1

Physical Properties

Property code	Value	Unit	Source
gf	-12.03	kJ/mol	Joback Method
hf	-354.51	kJ/mol	Joback Method
hfus	26.32	kJ/mol	Joback Method
hvap	73.01	kJ/mol	Joback Method
log10ws	-2.68		Crippen Method
logp	1.009		Crippen Method
mcvol	184.080	ml/mol	McGowan Method
pc	3284.05	kPa	Joback Method
rinpol	2085.00		NIST Webbook
rinpol	2085.00		NIST Webbook
tb	848.85	K	Joback Method
tc	1131.90	K	Joback Method
tf	721.21	K	Joback Method
vc	0.681	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	567.93	J/mol×K	848.85	Joback Method
cpg	585.76	J/mol×K	896.03	Joback Method
cpg	602.34	J/mol×K	943.20	Joback Method
cpg	617.70	J/mol×K	990.38	Joback Method

cpg	631.85	J/mol×K	1037.55	Joback Method
cpg	644.85	J/mol×K	1084.73	Joback Method
cpg	656.70	J/mol×K	1131.90	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=C52584391&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