5-Nonyl-5-ethylbarbituric acid

Inchi: InChI=1S/C15H26N2O3/c1-3-5-6-7-8-9-10-11-15(4-2)12(18)16-14(20)17-13(15)19/h3-11
InchiKey: KMXPZGOJCXKDSG-UHFFFAOYSA-N
Formula: C15H26N2O3
SMILES: CCCCCCCCCC1(CC)C(=O)NC(=O)NC1=O
Mol. weight [g/mol]: 282.38

Physical Properties

Property code	Value	Unit	Source
gf	-97.97	kJ/mol	Joback Method
hf	-620.85	kJ/mol	Joback Method
hfus	37.85	kJ/mol	Joback Method
hvap	74.52	kJ/mol	Joback Method
log10ws	-4.46		Aqueous and cosolvent solubility data for drug-like organic compounds
logp	2.889		Crippen Method
mcvol	236.020	ml/mol	McGowan Method
pc	1970.05	kPa	Joback Method
tb	862.95	K	Joback Method
tc	1094.68	K	Joback Method
tf	704.81	K	Joback Method
vc	0.901	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	781.77	J/mol×K	862.95	Joback Method
cpg	801.08	J/mol×K	901.57	Joback Method
cpg	819.30	J/mol×K	940.19	Joback Method
cpg	836.46	J/mol×K	978.81	Joback Method
cpg	852.58	J/mol×K	1017.44	Joback Method
cpg	867.70	J/mol×K	1056.06	Joback Method
cpg	881.83	J/mol×K	1094.68	Joback Method

Sources

Joback Method:	https://en.wikipedia.org/wiki/Joback_method
Aqueous and cosolvent solubility data for drug-like organic compounds:	https://www.ncbi.nlm.nih.gov/pmc/articles/PMC2751500/
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
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