Benzalbarbituric acid

Other names:	2,4,6(1H,3H,5H)-Pyrimidinetrione, 5-(phenylmethylene)-
	5-Benzylidenebarbituric acid
	5-Benzylidene-2,4,6(1H,3H,5H)-pyrimidinetrione
Inchi:	InChI=1S/C11H8N2O3/c14-9-8(10(15)13-11(16)12-9)6-7-4-2-1-3-5-7/h1-6H,(H2,12,13,14
InchiKey:	CMWDWOZYVQQAMI-UHFFFAOYSA-N
Formula:	C11H8N2O3
SMILES:	O=C1NC(=O)C(=Cc2ccccc2)C(=O)N1
Mol. weight [g/mol]:	216.19
CAS:	27402-47-7

Physical Properties

Property code	Value	Unit	Source
gf	39.42	kJ/mol	Joback Method
hf	-220.63	kJ/mol	Joback Method
hfus	27.08	kJ/mol	Joback Method
hvap	70.14	kJ/mol	Joback Method
log10ws	-2.13		Crippen Method
logp	0.436		Crippen Method
mcvol	151.600	ml/mol	McGowan Method
pc	4322.57	kPa	Joback Method
tb	809.18	K	Joback Method
tc	1103.33	K	Joback Method
tf	676.85	K	Joback Method
vc	0.555	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	430.05	J/mol×K	809.18	Joback Method
cpg	444.08	J/mol×K	858.20	Joback Method
cpg	456.06	J/mol×K	907.23	Joback Method
cpg	465.84	J/mol×K	956.25	Joback Method
cpg	473.25	J/mol×K	1005.28	Joback Method
cpg	478.15	J/mol×K	1054.30	Joback Method

cpg	480.37	J/mol×K	1103.33	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C27402477&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
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

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

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