BAMETHAN

Other names:	Benzenemethanol, «alpha»-[(butylamino)methyl]-4-hydroxy- Benzyl alcohol, «alpha»-((butylamino)methyl)-p-hydroxy- Bamethane Butedrine «alpha»-((Butylamino)methyl)-4-hydroxybenzenemethanol 2-Butylamino-1-p-hydroxyphenylethanol «alpha»-((Butylamino)methyl)-p-hydroxybenzyl alcohol N-Dutylnorsympathol Butyl-nor-sympatol N-Butylnorsynephrine Butylsympathol 1-(p-Hydroxyphenyl)-2-butylaminoethanol 1-(4-Hydroxyphenyl)-1-hydroxy-2-butylaminoethane «alpha»-[(Butylamino)methyl]-p-hydroxybenzyl, «alpha»-hydroxyl- (.+/-.)-Bamethane dl-Bamethane
Inchi:	InChI=1S/C12H19NO2/c1-2-3-8-13-9-12(15)10-4-6-11(14)7-5-10/h4-7,12-15H,2-3,8-9H2
InchiKey:	RDUHXGIIUDVSHR-UHFFFAOYSA-N
Formula:	C12H19NO2
SMILES:	CCCCNCC(O)c1ccc(O)cc1
Mol. weight [g/mol]:	209.29

Physical Properties

Property code	Value	Unit	Source
hf	-339.18	kJ/mol	Cheméo Relay (1.0)
hfus	32.32	kJ/mol	Joback Method
hvap	108.18	kJ/mol	Cheméo Relay (1.0)
ie	8.13	eV	Cheméo Relay (1.0)
log10ws	-0.51		Cheméo Relay (1.0)
logp	1.815		Crippen Method
mcvol	177.900	ml/mol	McGowan Method
rinpol	1735.00		NIST Webbook
tb	596.87	K	Cheméo Relay (1.0)
tf	402.88	K	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	512.35	J/mol×K	723.17	Joback Method
cpg	524.70	J/mol×K	756.83	Joback Method
cpg	536.38	J/mol×K	790.49	Joback Method
cpg	547.46	J/mol×K	824.15	Joback Method
cpg	558.01	J/mol×K	857.82	Joback Method
cpg	568.11	J/mol×K	891.48	Joback Method
cpg	577.83	J/mol×K	925.14	Joback Method

Sources

Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws
Cheméo Relay (1.0):
Cheméo Relay (1.0, beta):
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C3703795&Units=SI
Joback Method: https://en.wikipedia.org/wiki/Joback_method
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
hf: Enthalpy of formation at standard conditions
hfus: Enthalpy of fusion at standard conditions
hvap: Enthalpy of vaporization at standard conditions
ie: Ionization energy
log10ws: Log10 of Water solubility in mol/l
logp: Octanol/Water partition coefficient
mcvol: McGowan's characteristic volume
rinpol: Non-polar retention indices
tb: Normal Boiling Point Temperature
tf: Normal melting (fusion) point