

«beta»-Eucaïne

Other names:	Betacain Eucaïn B Eucaïne Eucaïne B 4-Piperidinol, 2,2,6-trimethyl-, benzoate (ester) 4-Piperidinol, 2,2,6-trimethyl-, benzoate (ester), stereoisomer 4-Piperidinol, 2,2,6-trimethyl-, benzoate Eukain B 2,2,6-Trimethyl-4-piperidinol benzoate (ester) Betacaine NSC 49860 4-Piperidinol, 2,2,6-trimethyl-, 4-benzoate Benzamine
Inchi:	InChI=1S/C15H21NO2/c1-11-9-13(10-15(2,3)16-11)18-14(17)12-7-5-4-6-8-12/h4-8,11,13
InchiKey:	ZYHGIAPHLSTGMX-UHFFFAOYSA-N
Formula:	C15H21NO2
SMILES:	<chem>CC1CC(OC(=O)c2ccccc2)CC(C)(C)N1</chem>
Mol. weight [g/mol]:	247.33
CAS:	500-34-5

Physical Properties

Property code	Value	Unit	Source
gf	45.16	kJ/mol	Joback Method
hf	-294.51	kJ/mol	Joback Method
hfus	28.70	kJ/mol	Joback Method
hvap	65.83	kJ/mol	Joback Method
log10ws	-4.06		Crippen Method
logp	2.763		Crippen Method
mcvol	205.010	ml/mol	McGowan Method
pc	2329.27	kPa	Joback Method
rinpola	1820.00		NIST Webbook
rinpola	1816.00		NIST Webbook
tb	704.57	K	Joback Method
tc	946.09	K	Joback Method
tf	485.22	K	Joback Method
vc	0.757	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	590.78	J/mol×K	704.57	Joback Method
cpg	611.20	J/mol×K	744.82	Joback Method
cpg	630.45	J/mol×K	785.08	Joback Method
cpg	648.67	J/mol×K	825.33	Joback Method
cpg	666.00	J/mol×K	865.59	Joback Method
cpg	682.57	J/mol×K	905.84	Joback Method
cpg	698.52	J/mol×K	946.09	Joback Method

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
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=C500345&Units=SI

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
rinpolar:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point

vc: Critical Volume

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