Bunolol

Inchi: InChI=1S/C17H25NO3/c1-17(2,3)18-10-12(19)11-21-16-9-5-6-13-14(16)7-4-8-15(13)20/h
InchiKey: IXHBTMCLRNMKHZ-LBPRGKRZSA-N
Formula: C17H25NO3
SMILES: CC(C)(C)NCC(O)COc1cccc2c1CCCC2=O
Mol. weight [g/mol]: 291.39
CAS: 27591-01-1

Physical Properties

Property code	Value	Unit	Source
gf	-32.85	kJ/mol	Joback Method
hf	-476.35	kJ/mol	Joback Method
hfus	26.96	kJ/mol	Joback Method
hvap	85.52	kJ/mol	Joback Method
log10ws	-4.14		Crippen Method
logp	2.333		Crippen Method
mcvol	239.060	ml/mol	McGowan Method
pc	2045.61	kPa	Joback Method
rinpol	2352.00		NIST Webbook
tb	869.60	K	Joback Method
tc	1088.20	K	Joback Method
tf	542.82	K	Joback Method
vc	0.891	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	774.65	J/mol×K	869.60	Joback Method
cpg	789.21	J/mol×K	906.03	Joback Method
cpg	802.67	J/mol×K	942.47	Joback Method
cpg	815.09	J/mol×K	978.90	Joback Method
cpg	826.51	J/mol×K	1015.33	Joback Method
cpg	837.00	J/mol×K	1051.77	Joback Method
cpg	846.61	J/mol×K	1088.20	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C27591011&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

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

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