Propranolol

Other names:	(.+/-.)-Propranolol
	(±) 1-(Isopropylamino)-3-(1-naphthyloxy)-2-propanol (propranolol)
	1-Isopropylamino-3-(1-naphthyloxy)-2-propanol
	2-Propanol, 1-(isopropylamino)-3-(1-naphthyloxy)-
	2-Propanol, 1-[(1-methylethyl)amino]-3-(1-naphthalenyloxy)-
	AY 64043
	Betalong
	DL-Propranolol
	Euprovasin
	Propanalol
	Propanolol
	Propranalol
	Proprasylyt
	Reducor
	Sawatal
	beta-Propranolol
	«beta»-Propranolol
Inchi:	InChI=1S/C16H21NO2/c1-12(2)17-10-14(18)11-19-16-9-5-7-13-6-3-4-8-15(13)16/h3-9,12
InchiKey:	AQHHHDLHHXJYJD-UHFFFAOYSA-N
Formula:	C16H21NO2
SMILES:	CC(C)NCC(O)COc1cccc2ccccc12
Mol. weight [g/mol]:	259.34
CAS:	525-66-6

Physical Properties

Property code	Value	Unit	Source
gf	135.96	kJ/mol	Joback Method
hf	-198.98	kJ/mol	Joback Method
hfus	31.20	kJ/mol	Joback Method
hvap	80.54	kJ/mol	Joback Method
log10ws	-3.49		Aqueous Solubility Prediction Method
logp	2.578		Crippen Method
mcvol	214.800	ml/mol	McGowan Method
pc	2291.52	kPa	Joback Method
rinpol	2152.00		NIST Webbook
rinpol	2139.00		NIST Webbook

rinpol	2141.00		NIST Webbook
rinpol	2141.00		NIST Webbook
rinpol	2150.00		NIST Webbook
rinpol	2142.00		NIST Webbook
rinpol	2136.00		NIST Webbook
rinpol	2138.00		NIST Webbook
rinpol	2111.00		NIST Webbook
rinpol	2155.00		NIST Webbook
rinpol	2157.00		NIST Webbook
rinpol	2152.00		NIST Webbook
rinpol	2157.00		NIST Webbook
rinpol	2141.00		NIST Webbook
rinpol	2150.00		NIST Webbook
rinpol	2142.00		NIST Webbook
rinpol	2133.00		NIST Webbook
rinpol	2136.00		NIST Webbook
tb	780.01	K	Joback Method
tc	987.06	K	Joback Method
tf	447.43	K	Joback Method
vc	0.805	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	694.04	J/mol×K	952.55	Joback Method
cpg	633.23	J/mol×K	780.01	Joback Method
cpg	647.05	J/mol×K	814.52	Joback Method
cpg	659.98	J/mol×K	849.03	Joback Method
cpg	672.09	J/mol×K	883.53	Joback Method
cpg	683.42	J/mol×K	918.04	Joback Method
cpg	704.00	J/mol×K	987.06	Joback Method
hfust	43.45	kJ/mol	365.50	NIST Webbook

Sources

Joback Method: https://en.wikipedia.org/wiki/Joback_method

Aqueous Solubility Prediction Method: http://onschallenge.wikispaces.com/file/view/AqueousDataset002.xlsx/351826032/AqueousDa

McGowan Method: http://link.springer.com/article/10.1007/BF02311772

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C525666&Units=SI
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
hfust:	Enthalpy of fusion at a given temperature
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