Toliprolol

Other names:	2-Propanol, 1-[(1-methylethyl)amino]-3-(3-methylphenoxy)-
	2-Propanol, 1-(isopropylamino)-3-(m-tolyloxy)-
	Isopropylamino-1-m-tolyloxy-3-propan-2-ol
	1-(Isopropylamino)-3-(m-tolyloxy)-2-propanol
	MHIP
	5711-18-2 (hydrochloride)
Inchi:	InChI=1S/C13H21NO2/c1-10(2)14-8-12(15)9-16-13-6-4-5-11(3)7-13/h4-7,10,12,14-15H,8
InchiKey:	NXQMNKUGGYNLBY-UHFFFAOYSA-N
Formula:	C13H21NO2
SMILES:	Cc1cccc(OCC(O)CNC(C)C)c1
Mol. weight [g/mol]:	223.31
CAS:	2933-94-0

Physical Properties

Property code	Value	Unit	Source
gf	4.05	kJ/mol	Joback Method
hf	-328.13	kJ/mol	Joback Method
hfus	26.41	kJ/mol	Joback Method
hvap	72.22	kJ/mol	Joback Method
log10ws	-2.84		Crippen Method
logp	1.733		Crippen Method
mcvol	191.990	ml/mol	McGowan Method
pc	2388.85	kPa	Joback Method
rinpol	1721.00		NIST Webbook
rinpol	1721.00		NIST Webbook
tb	692.39	K	Joback Method
tc	885.93	K	Joback Method
tf	380.92	K	Joback Method
vc	0.716	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	538.22	J/mol×K	692.39	Joback Method

cpg	552.46	J/mol×K	724.65	Joback Method
cpg	565.90	J/mol×K	756.90	Joback Method
cpg	578.56	J/mol×K	789.16	Joback Method
cpg	590.46	J/mol×K	821.42	Joback Method
cpg	601.62	J/mol×K	853.68	Joback Method
cpg	612.06	J/mol×K	885.93	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C2933940&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
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume