2-Propanol, 1-[(1-methylethyl)amino]-3-(1-naphthalenyloxy)-, (S)-

Other names: (S)-1-(isopropylamino)-3-(naphthyloxy)propan-2-ol
(-) 1-(Isopropylamino)-3-(1-naphthyloxy)-2-propanol (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-CQSZACIVSA-N

Formula: C16H21NO2

SMILES: CC(C)NCC(O)COc1cccc2ccccc12

Mol. weight [g/mol]: 259.34

CAS: 4199-09-1

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	-4.17		Crippen Method
logp	2.578		Crippen Method
mcvol	214.800	ml/mol	McGowan Method
pc	2291.52	kPa	Joback Method
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	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	694.04	J/mol×K	952.55	Joback Method
cpg	704.00	J/mol×K	987.06	Joback Method

hfust	36.25	kJ/mol	344.70	NIST Webbook

Sources

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=C4199091&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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume