occidentalol

Inchi: InChI=1S/C15H24O/c1-11-6-5-8-15(4)9-7-12(10-13(11)15)14(2,3)16/h5-6,8,12-13,16H,7
InchiKey: AMZWKSYAMHGGSR-GZBFAFLISA-N
Formula: C15H24O
SMILES: CC1=CC=CC2(C)CCC(C(C)(C)O)CC12
Mol. weight [g/mol]: 220.35
CAS: 473-17-6

Physical Properties

Property code	Value	Unit	Source
gf	51.63	kJ/mol	Joback Method
hf	-293.96	kJ/mol	Joback Method
hfus	15.98	kJ/mol	Joback Method
hvap	64.67	kJ/mol	Joback Method
log10ws	-4.25		Crippen Method
logp	3.696		Crippen Method
mcvol	197.760	ml/mol	McGowan Method
pc	2229.20	kPa	Joback Method
rinpol	1548.00		NIST Webbook
rinpol	1548.00		NIST Webbook
rinpol	1538.00		NIST Webbook
rinpol	1545.00		NIST Webbook
ripol	2086.00		NIST Webbook
ripol	2097.00		NIST Webbook
ripol	2097.00		NIST Webbook
tb	660.98	K	Joback Method
tc	875.00	K	Joback Method
tf	377.55	K	Joback Method
vc	0.735	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	575.18	J/mol×K	660.98	Joback Method
cpg	594.14	J/mol×K	696.65	Joback Method

cpg	612.03	J/mol×K	732.32	Joback Method
cpg	629.01	J/mol×K	767.99	Joback Method
cpg	645.25	J/mol×K	803.66	Joback Method
cpg	660.89	J/mol×K	839.33	Joback Method
cpg	676.10	J/mol×K	875.00	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C473176&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
ripol:	Polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume