Exaprolol

Inchi: InChI=1S/C18H29NO2/c1-14(2)19-12-16(20)13-21-18-11-7-6-10-17(18)15-8-4-3-5-9-15/h
InchiKey: ABXHHEZNIJUQFM-UHFFFAOYSA-N
Formula: C18H29NO2
SMILES: CC(C)NCC(O)COc1ccccc1C1CCCCC1
Mol. weight [g/mol]: 291.43

Physical Properties

Property code	Value	Unit	Source
gf	70.60	kJ/mol	Joback Method
hf	-377.01	kJ/mol	Joback Method
hfus	31.19	kJ/mol	Joback Method
hvap	83.78	kJ/mol	Joback Method
log10ws	-4.70		Crippen Method
logp	3.472		Crippen Method
mcvol	251.580	ml/mol	McGowan Method
pc	1856.31	kPa	Joback Method
rinpol	2169.00		NIST Webbook
rinpol	2169.00		NIST Webbook
tb	826.34	K	Joback Method
tc	1036.44	K	Joback Method
tf	444.65	K	Joback Method
vc	0.928	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	813.39	J/mol×K	826.34	Joback Method
cpg	830.57	J/mol×K	861.36	Joback Method
cpg	846.49	J/mol×K	896.37	Joback Method
cpg	861.18	J/mol×K	931.39	Joback Method
cpg	874.70	J/mol×K	966.40	Joback Method
cpg	887.09	J/mol×K	1001.42	Joback Method
cpg	898.40	J/mol×K	1036.44	Joback Method

Sources

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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R217868&Units=SI

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