Oligandrol

Inchi: InChI=1S/C22H32O2/c1-16(2)8-6-9-17(3)10-7-12-22(5)13-11-19-15-20(23)14-18(4)21(19
InchiKey: OJZATKPMGAGZGS-LICLKQGHSA-N
Formula: C22H32O2
SMILES: CC(C)=CCCC(C)=CCCC1(C)CCc2cc(O)cc(C)c2O1
Mol. weight [g/mol]: 328.49
CAS: 155661-15-7

Physical Properties

Property code	Value	Unit	Source
gf	173.27	kJ/mol	Joback Method
hf	-296.39	kJ/mol	Joback Method
hfus	47.28	kJ/mol	Joback Method
hvap	84.70	kJ/mol	Joback Method
log10ws	-7.15		Crippen Method
logp	6.257		Crippen Method
mcvol	289.360	ml/mol	McGowan Method
pc	1508.15	kPa	Joback Method
rinpol	2710.30		NIST Webbook
rinpol	2710.30		NIST Webbook
tb	866.30	K	Joback Method
tc	1092.99	K	Joback Method
tf	527.69	K	Joback Method
vc	1.056	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	922.89	J/mol×K	866.30	Joback Method
cpg	944.09	J/mol×K	904.08	Joback Method
cpg	965.35	J/mol×K	941.86	Joback Method
cpg	986.94	J/mol×K	979.65	Joback Method
cpg	1009.13	J/mol×K	1017.43	Joback Method
cpg	1032.18	J/mol×K	1055.21	Joback Method
cpg	1056.35	J/mol×K	1092.99	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C155661157&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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume