Illidol

Inchi: InChI=1S/C15H26O3/c1-14(2)5-8-11(6-14)15(3)10(4-12(15)17)9(7-16)13(8)18/h8-13,16-
InchiKey: HNXKXCUDHZKBFM-LBTGFFJWSA-N
Formula: C15H26O3
SMILES: CC1(C)CC2C(O)C(CO)C3CC(O)C3(C)C2C1
Mol. weight [g/mol]: 254.37

Physical Properties

Property code	Value	Unit	Source
gf	-226.52	kJ/mol	Joback Method
hf	-674.76	kJ/mol	Joback Method
hfus	29.83	kJ/mol	Joback Method
hvap	95.26	kJ/mol	Joback Method
log10ws	-2.35		Crippen Method
logp	1.409		Crippen Method
mcvol	207.240	ml/mol	McGowan Method
pc	2458.04	kPa	Joback Method
rinpol	1589.00		NIST Webbook
tb	825.03	K	Joback Method
tc	1019.60	K	Joback Method
tf	514.65	K	Joback Method
vc	0.778	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	742.25	J/mol×K	825.03	Joback Method
cpg	759.67	J/mol×K	857.46	Joback Method
cpg	777.20	J/mol×K	889.89	Joback Method
cpg	795.01	J/mol×K	922.32	Joback Method
cpg	813.29	J/mol×K	954.75	Joback Method
cpg	832.22	J/mol×K	987.17	Joback Method
cpg	851.99	J/mol×K	1019.60	Joback Method

Sources

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=R617817&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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