Jinkho-eremol

Inchi: InChI=1S/C15H26O/c1-11-6-5-7-12-8-9-13(14(2,3)16)10-15(11,12)4/h5,7,11-13,16H,6,8-
InchiKey: STRWISYROJVASE-YKURLNKLSA-N
Formula: C15H26O
SMILES: CC1CC=CC2CCC(C(C)(C)O)CC12C
Mol. weight [g/mol]: 222.37

Physical Properties

Property code	Value	Unit	Source
gf	23.59	kJ/mol	Joback Method
hf	-360.61	kJ/mol	Joback Method
hfus	16.22	kJ/mol	Joback Method
hvap	63.40	kJ/mol	Joback Method
log10ws	-4.15		Crippen Method
logp	3.776		Crippen Method
mcvol	202.060	ml/mol	McGowan Method
pc	2119.73	kPa	Joback Method
rinpol	1642.00		NIST Webbook
rinpol	1643.00		NIST Webbook
tb	652.17	K	Joback Method
tc	863.51	K	Joback Method
tf	360.03	K	Joback Method
vc	0.748	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	599.78	J/mol×K	652.17	Joback Method
cpg	620.42	J/mol×K	687.39	Joback Method
cpg	639.88	J/mol×K	722.62	Joback Method
cpg	658.32	J/mol×K	757.84	Joback Method
cpg	675.87	J/mol×K	793.06	Joback Method
cpg	692.70	J/mol×K	828.29	Joback Method
cpg	708.96	J/mol×K	863.51	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R613033&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
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

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