DehydroJinkho-eremol

Inchi: InChI=1S/C15H24O/c1-11-6-5-7-12-8-9-13(14(2,3)16)10-15(11,12)4/h5,7-9,11-13,16H,6,
InchiKey: RBXTWLKVKMWZLA-YKURLNKLSA-N
Formula: C15H24O
SMILES: CC1CC=CC2C=CC(C(C)(C)O)CC21C
Mol. weight [g/mol]: 220.35

Physical Properties

Property code	Value	Unit	Source
gf	53.55	kJ/mol	Joback Method
hf	-302.83	kJ/mol	Joback Method
hfus	17.44	kJ/mol	Joback Method
hvap	63.70	kJ/mol	Joback Method
log10ws	-4.01		Crippen Method
logp	3.552		Crippen Method
mcvol	197.760	ml/mol	McGowan Method
pc	2191.78	kPa	Joback Method
rinpol	1674.00		NIST Webbook
rinpol	1673.00		NIST Webbook
tb	651.33	K	Joback Method
tc	864.46	K	Joback Method
tf	360.79	K	Joback Method
vc	0.734	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	577.13	J/mol×K	651.33	Joback Method
cpg	596.79	J/mol×K	686.85	Joback Method
cpg	615.30	J/mol×K	722.37	Joback Method
cpg	632.82	J/mol×K	757.89	Joback Method
cpg	649.50	J/mol×K	793.42	Joback Method
cpg	665.50	J/mol×K	828.94	Joback Method
cpg	680.98	J/mol×K	864.46	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R612976&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