

Incisol

Inchi:	InChI=1S/C15H24O/c1-6-15(5)13(9-7-11(2)3)12(4)8-10-14(15)16/h6-7,9,11,13-14,16H,1
InchiKey:	DXMDZNOPRIYRBA-DKZXYHOFSA-N
Formula:	C15H24O
SMILES:	<chem>C=CC1(C)C(O)CCC(=C)C1C=CC(C)C</chem>
Mol. weight [g/mol]:	220.35

Physical Properties

Property code	Value	Unit	Source
gf	160.84	kJ/mol	Joback Method
hf	-154.67	kJ/mol	Joback Method
hfus	20.61	kJ/mol	Joback Method
hvap	63.38	kJ/mol	Joback Method
log10ws	-4.21		Crippen Method
logp	3.718		Crippen Method
mcvol	204.320	ml/mol	McGowan Method
pc	1956.14	kPa	Joback Method
rinsol	1540.00		NIST Webbook
tb	644.79	K	Joback Method
tc	841.81	K	Joback Method
tf	334.27	K	Joback Method
vc	0.762	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	564.24	J/mol×K	644.79	Joback Method
cpg	582.12	J/mol×K	677.63	Joback Method
cpg	599.14	J/mol×K	710.46	Joback Method
cpg	615.38	J/mol×K	743.30	Joback Method
cpg	630.96	J/mol×K	776.14	Joback Method
cpg	645.98	J/mol×K	808.97	Joback Method
cpg	660.52	J/mol×K	841.81	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=R440543&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
hvac:	Enthalpy of vaporization at standard conditions
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mccol:	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

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