Italicen-12-ol

Inchi: InChI=1S/C15H24O/c1-10-6-7-15-11(2)4-5-12(15)14(3,9-16)13(15)8-10/h8,11-13,16H,4-
InchiKey: MNQNDAQBBYTPHH-QTVXIADOSA-N
Formula: C15H24O
SMILES: CC1=CC2C(C)(CO)C3CCC(C)C23CC1
Mol. weight [g/mol]: 220.35

Physical Properties

Property code	Value	Unit	Source
gf	90.58	kJ/mol	Joback Method
hf	-262.97	kJ/mol	Joback Method
hfus	19.28	kJ/mol	Joback Method
hvap	63.78	kJ/mol	Joback Method
log10ws	-3.69		Crippen Method
logp	3.387		Crippen Method
mcvol	191.200	ml/mol	McGowan Method
pc	2309.17	kPa	Joback Method
rinpol	1662.00		NIST Webbook
tb	658.82	K	Joback Method
tc	867.61	K	Joback Method
tf	419.01	K	Joback Method
vc	0.730	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	574.50	J/mol×K	658.82	Joback Method
cpg	592.95	J/mol×K	693.62	Joback Method
cpg	610.61	J/mol×K	728.42	Joback Method
cpg	627.74	J/mol×K	763.22	Joback Method
cpg	644.56	J/mol×K	798.01	Joback Method
cpg	661.31	J/mol×K	832.81	Joback Method
cpg	678.22	J/mol×K	867.61	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=R233142&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

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