Isovalencenol

Inchi: InChI=1S/C15H24O/c1-11(10-16)13-7-8-14-6-4-5-12(2)15(14,3)9-13/h6,9,11-12,16H,4-5
InchiKey: MCDRFHDZJOGPFL-WQKBPTQTSA-N
Formula: C15H24O
SMILES: CC(CO)C1=CC2(C)C(=CCCC2C)CC1
Mol. weight [g/mol]: 220.35

Physical Properties

Property code	Value	Unit	Source
gf	44.43	kJ/mol	Joback Method
hf	-281.62	kJ/mol	Joback Method
hfus	18.41	kJ/mol	Joback Method
hvap	66.55	kJ/mol	Joback Method
log10ws	-4.14		Crippen Method
logp	3.698		Crippen Method
mcvol	197.760	ml/mol	McGowan Method
pc	2244.00	kPa	Joback Method
rinpol	1775.00		NIST Webbook
rinpol	1813.00		NIST Webbook
ripol	2555.00		NIST Webbook
tb	673.42	K	Joback Method
tc	881.23	K	Joback Method
tf	376.89	K	Joback Method
vc	0.741	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	570.73	J/mol×K	673.42	Joback Method
cpg	588.67	J/mol×K	708.05	Joback Method
cpg	605.74	J/mol×K	742.69	Joback Method
cpg	622.06	J/mol×K	777.32	Joback Method
cpg	637.76	J/mol×K	811.96	Joback Method
cpg	652.96	J/mol×K	846.59	Joback Method
cpg	667.80	J/mol×K	881.23	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=R341194&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
ripol:	Polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume