Isorotundene

Inchi: InChI=1S/C15H24/c1-10-4-5-14-13(10)8-12-6-7-15(14,3)9-11(12)2/h10,12-14H,2,4-9H2,1
InchiKey: NPHFULIVCUBDDN-HUGQBSPZSA-N
Formula: C15H24
SMILES: C=C1CC2(C)CCC1CC1C(C)CCC12
Mol. weight [g/mol]: 204.35

Physical Properties

Property code	Value	Unit	Source
gf	253.54	kJ/mol	Joback Method
hf	-94.21	kJ/mol	Joback Method
hfus	17.40	kJ/mol	Joback Method
hvap	47.63	kJ/mol	Joback Method
log10ws	-4.43		Crippen Method
logp	4.415		Crippen Method
mcvol	185.330	ml/mol	McGowan Method
pc	2075.54	kPa	Joback Method
rinpol	1560.00		NIST Webbook
rinpol	1560.00		NIST Webbook
tb	565.69	K	Joback Method
tc	788.81	K	Joback Method
tf	331.17	K	Joback Method
vc	0.703	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	504.76	J/mol×K	565.69	Joback Method
cpg	529.18	J/mol×K	602.88	Joback Method
cpg	552.00	J/mol×K	640.06	Joback Method
cpg	573.39	J/mol×K	677.25	Joback Method
cpg	593.54	J/mol×K	714.44	Joback Method
cpg	612.64	J/mol×K	751.63	Joback Method
cpg	630.85	J/mol×K	788.81	Joback Method

Sources

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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R621059&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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