Rotundene

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-ZNDVUOBYSA-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	1469.00		NIST Webbook
rinpol	1466.00		NIST Webbook
rinpol	1469.00		NIST Webbook
rinpol	1460.00		NIST Webbook
rinpol	1461.00		NIST Webbook
rinpol	1469.00		NIST Webbook
rinpol	1460.00		NIST Webbook
rinpol	1462.00		NIST Webbook
ripol	1629.00		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

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=R285524&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