

«gamma»-Acoradiene

Inchi:

InChI=1S/C15H24/c1-11(2)14-6-5-13(4)15(14)9-7-12(3)8-10-15/h7,13H,5-6,8-10H2,1-4H

InchiKey:

HMKLOOMRRZKSNM-UKRRQHHQSA-N

Formula:

C15H24

SMILES:

CC1=CCC2(CC1)C(=C(C)C)CCC2C

Mol. weight [g/mol]:

204.35

Physical Properties

Property code	Value	Unit	Source
gf	200.27	kJ/mol	Joback Method
hf	-104.18	kJ/mol	Joback Method
hfus	16.02	kJ/mol	Joback Method
hvap	50.17	kJ/mol	Joback Method
log10ws	-5.11		Crippen Method
logp	4.869		Crippen Method
mcvol	191.890	ml/mol	McGowan Method
pc	2069.88	kPa	Joback Method
rinpol	1513.00		NIST Webbook
rinpol	1513.00		NIST Webbook
ripol	1689.00		NIST Webbook
tb	584.06	K	Joback Method
tc	811.24	K	Joback Method
tf	314.19	K	Joback Method
vc	0.726	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	501.06	J/mol×K	584.06	Joback Method
cpg	523.47	J/mol×K	621.92	Joback Method
cpg	544.48	J/mol×K	659.79	Joback Method
cpg	564.25	J/mol×K	697.65	Joback Method
cpg	582.97	J/mol×K	735.51	Joback Method
cpg	600.80	J/mol×K	773.38	Joback Method
cpg	617.92	J/mol×K	811.24	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R613484&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307I
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

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
rlnpol:	Non-polar retention indices
ripol:	Polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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