

5-(1,5-Dimethyl-1,4-hexadienyl)-tetrahydro-2-meth

Inchi:	InChI=1S/C15H24O/c1-6-15(5)11-10-14(16-15)13(4)9-7-8-12(2)3/h6,8-9,14H,1,7,10-11H
InchiKey:	SADCLHOFZYXXAL-UKTHLTGXSA-N
Formula:	C15H24O
SMILES:	<chem>C=CC1(C)CCC(C(C)=CCC=C(C)C)O1</chem>
Mol. weight [g/mol]:	220.35

Physical Properties

Property code	Value	Unit	Source
gf	243.83	kJ/mol	Joback Method
hf	-89.26	kJ/mol	Joback Method
hfus	27.80	kJ/mol	Joback Method
hvap	51.70	kJ/mol	Joback Method
log10ws	-4.87		Crippen Method
logp	4.413		Crippen Method
mvol	204.320	ml/mol	McGowan Method
pc	1859.51	kPa	Joback Method
tb	585.16	K	Joback Method
tc	797.12	K	Joback Method
tf	276.10	K	Joback Method
vc	0.777	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	526.25	J/molxK	585.16	Joback Method
cpg	546.63	J/molxK	620.49	Joback Method
cpg	565.78	J/molxK	655.81	Joback Method
cpg	583.85	J/molxK	691.14	Joback Method
cpg	601.01	J/molxK	726.47	Joback Method
cpg	617.41	J/molxK	761.79	Joback Method
cpg	633.19	J/molxK	797.12	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=R547689&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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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