

(R,Z)-2-Methyl-6-(4-methylcyclohexa-1,4-dien-1-yl)

Inchi:

InchiKey:

Formula:

SMILES:

Mol. weight [g/mol]:

CAS:

InChI=1S/C15H24O/c1-12-7-9-15(10-8-12)14(3)6-4-5-13(2)11-16/h5,7,10,14,16H,4,6,8-9

ZHWZEHFYKZGQFR-UUSOHVMFSA-N

C15H24O

CC(=CCCC(C)C1=CCC(C)=CC1)CO

220.35

698365-10-5

Physical Properties

Property code	Value	Unit	Source
gf	80.65	kJ/mol	Joback Method
hf	-235.73	kJ/mol	Joback Method
hfus	26.49	kJ/mol	Joback Method
hvap	67.96	kJ/mol	Joback Method
log10ws	-4.58		Crippen Method
logp	4.008		Crippen Method
mcvol	204.320	ml/mol	McGowan Method
pc	2027.23	kPa	Joback Method
rinpol	1730.00		NIST Webbook
rinpol	1761.20		NIST Webbook
rinpol	1761.20		NIST Webbook
tb	670.88	K	Joback Method
tc	865.17	K	Joback Method
tf	323.77	K	Joback Method
vc	0.775	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	562.11	J/molxK	670.88	Joback Method
cpg	578.29	J/molxK	703.26	Joback Method
cpg	593.59	J/molxK	735.64	Joback Method
cpg	608.05	J/molxK	768.02	Joback Method
cpg	621.72	J/molxK	800.40	Joback Method
cpg	634.65	J/molxK	832.79	Joback Method

Sources

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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C698365105&Units=SI

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

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