

2,5-Cyclohexadien-1-ol, 5-methyl-2-(1-methylethyl)

Inchi:	InChI=1S/C10H16O/c1-7(2)9-5-4-8(3)6-10(9)11/h5-7,10-11H,4H2,1-3H3
InchiKey:	PKASTMBNAVFTIZ-UHFFFAOYSA-N
Formula:	C10H16O
SMILES:	CC1=CC(O)C(C(C)C)=CC1
Mol. weight [g/mol]:	152.23

Physical Properties

Property code	Value	Unit	Source
gf	-40.83	kJ/mol	Joback Method
hf	-260.30	kJ/mol	Joback Method
hfus	15.72	kJ/mol	Joback Method
hvap	56.48	kJ/mol	Joback Method
log10ws	-2.74		Crippen Method
logp	2.280		Crippen Method
mcvol	138.170	ml/mol	McGowan Method
pc	2982.79	kPa	Joback Method
rinpol	1156.00		NIST Webbook
tb	547.77	K	Joback Method
tc	743.24	K	Joback Method
tf	282.22	K	Joback Method
vc	0.513	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	332.07	J/mol×K	547.77	Joback Method
cpg	346.08	J/mol×K	580.35	Joback Method
cpg	359.40	J/mol×K	612.93	Joback Method
cpg	372.05	J/mol×K	645.51	Joback Method
cpg	384.03	J/mol×K	678.09	Joback Method
cpg	395.38	J/mol×K	710.66	Joback Method
cpg	406.10	J/mol×K	743.24	Joback Method
dvisc	0.0140010	Paxs	282.22	Joback Method
dvisc	0.0035791	Paxs	326.48	Joback Method

dvisc	0.0012671	Paxs	370.74	Joback Method
dvisc	0.0005598	Paxs	415.00	Joback Method
dvisc	0.0002895	Paxs	459.25	Joback Method
dvisc	0.0001681	Paxs	503.51	Joback Method
dvisc	0.0001066	Paxs	547.77	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=R31789&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

Legend

cpg:	Ideal gas heat capacity
dvisc:	Dynamic viscosity
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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