

p-Mentha-1,5-dien-7-al

Other names:	«alpha»-Phellandral
Inchi:	InChI=1S/C10H14O/c1-8(2)10-5-3-9(7-11)4-6-10/h3-5,7-8,10H,6H2,1-2H3
InchiKey:	IHMUIEIWVVHVHY-UHFFFAOYSA-N
Formula:	C10H14O
SMILES:	CC(C)C1C=CC(C=O)=CC1
Mol. weight [g/mol]:	150.22

Physical Properties

Property code	Value	Unit	Source
gf	6.10	kJ/mol	Joback Method
hf	-182.18	kJ/mol	Joback Method
hfus	14.31	kJ/mol	Joback Method
hvap	45.86	kJ/mol	Joback Method
log10ws	-2.41		Crippen Method
logp	2.344		Crippen Method
mcvol	133.870	ml/mol	McGowan Method
pc	2973.04	kPa	Joback Method
tb	499.27	K	Joback Method
tc	711.26	K	Joback Method
tf	250.88	K	Joback Method
vc	0.511	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	295.92	J/molxK	499.27	Joback Method
cpg	365.53	J/molxK	675.93	Joback Method
cpg	353.24	J/molxK	640.60	Joback Method
cpg	340.15	J/molxK	605.26	Joback Method
cpg	326.26	J/molxK	569.93	Joback Method
cpg	311.52	J/molxK	534.60	Joback Method
cpg	377.06	J/molxK	711.26	Joback Method
dvisc	0.0002850	Paxs	499.27	Joback Method
dvisc	0.0003649	Paxs	457.87	Joback Method

dvisc	0.0004906	Paxs	416.47	Joback Method
dvisc	0.0007043	Paxs	375.07	Joback Method
dvisc	0.0011058	Paxs	333.68	Joback Method
dvisc	0.0019730	Paxs	292.28	Joback Method
dvisc	0.0042616	Paxs	250.88	Joback Method

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
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=R234472&Units=SI

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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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