1-phellandrene

Other names:	(R)-5-isopropyl-2-methylcyclohexa-1,3-diene
	1,3-Cyclohexadiene, 2-methyl-5-(1-methylethyl)-, (r)-
Inchi:	InChI=1S/C10H16/c1-8(2)10-6-4-9(3)5-7-10/h4-6,8,10H,7H2,1-3H3/t10-/m0/s1
InchiKey:	OGLDWXZKYODSOB-JTQLQIEISA-N
Formula:	C10H16
SMILES:	CC1=CCC(C(C)C)C=C1
Mol. weight [g/mol]:	136.23
CAS:	4221-98-1

Physical Properties

Property code	Value	Unit	Source
chl	-6014.10	kJ/mol	NIST Webbook
chl	-6013.20	kJ/mol	NIST Webbook
gf	105.62	kJ/mol	Joback Method
hf	-96.60	kJ/mol	Joback Method
hfus	12.02	kJ/mol	Joback Method
hvap	46.90	kJ/mol	NIST Webbook
hvap	48.30	kJ/mol	NIST Webbook
log10ws	-3.13		Crippen Method
logp	3.165		Crippen Method
mcvol	132.300	ml/mol	McGowan Method
pc	2746.90	kPa	Joback Method
rinpol	1012.00		NIST Webbook
rinpol	999.00		NIST Webbook
rinpol	992.00		NIST Webbook
rinpol	1012.00		NIST Webbook
ripol	1159.00		NIST Webbook
ripol	1159.00		NIST Webbook
ripol	1154.00		NIST Webbook
tb	450.61	K	Joback Method
tc	657.58	K	Joback Method
tf	208.88	K	Joback Method
vc	0.494	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	271.83	J/mol×K	450.61	Joback Method
cpg	349.14	J/mol×K	623.09	Joback Method
cpg	335.32	J/mol×K	588.59	Joback Method
cpg	320.71	J/mol×K	554.10	Joback Method
cpg	305.27	J/mol×K	519.60	Joback Method
cpg	288.98	J/mol×K	485.11	Joback Method
cpg	362.19	J/mol×K	657.58	Joback Method
dvisc	0.0002251	Pa×s	450.61	Joback Method
dvisc	0.0002905	Pa×s	410.32	Joback Method
dvisc	0.0003964	Pa×s	370.03	Joback Method
dvisc	0.0005836	Pa×s	329.75	Joback Method
dvisc	0.0009568	Pa×s	289.46	Joback Method
dvisc	0.0018408	Pa×s	249.17	Joback Method
dvisc	0.0045582	Pa×s	208.88	Joback Method

Sources

McGowan Method: http://link.springer.com/article/10.1007/BF02311772
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C4221981&Units=SI
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws
Joback Method: https://en.wikipedia.org/wiki/Joback_method

Legend

chl: Standard liquid enthalpy of combustion
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
ripol:	Polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume