(+)-«alpha»-phellandrene

Other names: (S)-2-methyl-5-(1-methylethyl)-1,3-cyclohexadiene
Inchi: InChI=1S/C10H16/c1-8(2)10-6-4-9(3)5-7-10/h4-6,8,10H,7H2,1-3H3/t10-/m1/s1
InchiKey: OGLDWXZKYODSOB-SNVBAGLBSA-N
Formula: C10H16
SMILES: CC1=CCC(C(C)C)C=C1
Mol. weight [g/mol]: 136.23
CAS: 2243-33-6

Physical Properties

Property code	Value	Unit	Source
gf	105.62	kJ/mol	Joback Method
hf	-96.60	kJ/mol	Joback Method
hfus	12.02	kJ/mol	Joback Method
hvap	39.14	kJ/mol	Joback Method
log10ws	-3.13		Crippen Method
logp	3.165		Crippen Method
mcvol	132.300	ml/mol	McGowan Method
pc	2746.90	kPa	Joback Method
rinpol	1006.00		NIST Webbook
rinpol	1006.00		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	288.98	J/mol×K	485.11	Joback Method
cpg	305.27	J/mol×K	519.60	Joback Method
cpg	320.71	J/mol×K	554.10	Joback Method
cpg	335.32	J/mol×K	588.59	Joback Method
cpg	349.14	J/mol×K	623.09	Joback Method

cpg	362.19	J/mol×K	657.58	Joback Method
dvisc	0.0045582	Pa×s	208.88	Joback Method
dvisc	0.0018408	Pa×s	249.17	Joback Method
dvisc	0.0009568	Pa×s	289.46	Joback Method
dvisc	0.0005836	Pa×s	329.75	Joback Method
dvisc	0.0003964	Pa×s	370.03	Joback Method
dvisc	0.0002905	Pa×s	410.32	Joback Method
dvisc	0.0002251	Pa×s	450.61	Joback Method

Sources

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
McGowan Method: http://link.springer.com/article/10.1007/BF02311772
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C2243336&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
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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