

«delta»-phellandrene

Inchi:	InChI=1S/C10H16/c1-8(2)10-6-4-9(3)5-7-10/h4,6,8,10H,3,5,7H2,1-2H3/t10-/m0/s1
InchiKey:	LFJQCDVYDGGFCH-JTQLQIEISA-N
Formula:	C10H16
SMILES:	C=C1C=CC(C(C)C)CC1
Mol. weight [g/mol]:	136.23

Physical Properties

Property code	Value	Unit	Source
gf	138.37	kJ/mol	Joback Method
hf	-58.67	kJ/mol	Joback Method
hfus	10.03	kJ/mol	Joback Method
hvap	38.35	kJ/mol	Joback Method
log10ws	-3.13		Crippen Method
logp	3.165		Crippen Method
mcvol	132.300	ml/mol	McGowan Method
pc	2741.15	kPa	Joback Method
rinpol	1026.00		NIST Webbook
rinpol	987.00		NIST Webbook
rinpol	1026.00		NIST Webbook
tb	445.63	K	Joback Method
tc	651.00	K	Joback Method
tf	209.28	K	Joback Method
vc	0.492	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	270.36	J/mol×K	445.63	Joback Method
cpg	287.65	J/mol×K	479.86	Joback Method
cpg	304.09	J/mol×K	514.09	Joback Method
cpg	319.70	J/mol×K	548.32	Joback Method
cpg	334.48	J/mol×K	582.55	Joback Method
cpg	348.47	J/mol×K	616.77	Joback Method
cpg	361.70	J/mol×K	651.00	Joback Method

dvisc	0.0047798	Paxs	209.28	Joback Method
dvisc	0.0019776	Paxs	248.67	Joback Method
dvisc	0.0010415	Paxs	288.06	Joback Method
dvisc	0.0006401	Paxs	327.45	Joback Method
dvisc	0.0004367	Paxs	366.85	Joback Method
dvisc	0.0003209	Paxs	406.24	Joback Method
dvisc	0.0002490	Paxs	445.63	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R231146&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

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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