

«beta»-Phellandren-6-ol

Inchi:	InChI=1S/C10H16O/c1-7(2)9-5-4-8(3)10(11)6-9/h4-5,7,9-11H,3,6H2,1-2H3/t9-,10?/m0/s
InchiKey:	VKAGFXRPRUAOHV-RGURZIINSA-N
Formula:	C10H16O
SMILES:	C=C1C=CC(C(C)C)CC1O
Mol. weight [g/mol]:	152.23

Physical Properties

Property code	Value	Unit	Source
gf	-6.16	kJ/mol	Joback Method
hf	-231.24	kJ/mol	Joback Method
hfus	15.19	kJ/mol	Joback Method
hvap	54.72	kJ/mol	Joback Method
log10ws	-2.50		Crippen Method
logp	2.136		Crippen Method
mcvol	138.170	ml/mol	McGowan Method
pc	2918.68	kPa	Joback Method
ripol	1196.00		NIST Webbook
ripol	1796.00		NIST Webbook
ripol	1796.00		NIST Webbook
tb	533.14	K	Joback Method
tc	726.14	K	Joback Method
tf	265.86	K	Joback Method
vc	0.510	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	332.43	J/mol×K	533.14	Joback Method
cpg	399.57	J/mol×K	693.98	Joback Method
cpg	387.52	J/mol×K	661.81	Joback Method
cpg	374.81	J/mol×K	629.64	Joback Method
cpg	361.39	J/mol×K	597.47	Joback Method
cpg	347.27	J/mol×K	565.31	Joback Method
cpg	410.94	J/mol×K	726.14	Joback Method

dvisc	0.0001414	Paxs	533.14	Joback Method
dvisc	0.0002220	Paxs	488.59	Joback Method
dvisc	0.0003816	Paxs	444.05	Joback Method
dvisc	0.0007401	Paxs	399.50	Joback Method
dvisc	0.0016951	Paxs	354.95	Joback Method
dvisc	0.0049246	Paxs	310.41	Joback Method
dvisc	0.0204533	Paxs	265.86	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R545618&Units=SI
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

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
mvol:	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

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