Dihydro-myrcenol acetate

Inchi: InChI=1S/C12H22O2/c1-6-10(2)8-7-9-12(4,5)14-11(3)13/h2,6-9H2,1,3-5H3
InchiKey: VHVRYMDFTKNLFA-UHFFFAOYSA-N
Formula: C12H22O2
SMILES: C=C(CC)CCCC(C)(C)OC(C)=O
Mol. weight [g/mol]: 198.30

Physical Properties

Property code	Value	Unit	Source
gf	-101.63	kJ/mol	Joback Method
hf	-428.92	kJ/mol	Joback Method
hfus	19.62	kJ/mol	Joback Method
hvap	49.58	kJ/mol	Joback Method
log10ws	-3.67		Crippen Method
logp	3.465		Crippen Method
mcvol	183.080	ml/mol	McGowan Method
pc	1961.34	kPa	Joback Method
rinpol	1214.00		NIST Webbook
rinpol	1214.00		NIST Webbook
tb	543.58	K	Joback Method
tc	728.61	K	Joback Method
tf	283.86	K	Joback Method
vc	0.703	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	447.13	J/mol×K	543.58	Joback Method
cpg	463.44	J/mol×K	574.42	Joback Method
cpg	478.95	J/mol×K	605.26	Joback Method
cpg	493.68	J/mol×K	636.10	Joback Method
cpg	507.66	J/mol×K	666.93	Joback Method
cpg	520.92	J/mol×K	697.77	Joback Method
cpg	533.49	J/mol×K	728.61	Joback Method

Sources

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=R232030&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

Legend

cpg:	Ideal gas heat capacity
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

Latest version available from:
https://www.chemeo.com/cid/85-068-3/Dihydro-myrcenol-acetate.pdf
Generated by Cheméo on 2025-12-23 09:49:22.50322269 +0000 UTC m=+6231560.033263344.
Cheméo (https://www.chemeo.com) is the biggest free database of chemical and physical data for the process industry.