Manool (epi-13)

Other names: 13-epi-Manool, isomer
Inchi: InChI=1S/C20H34O/c1-7-19(5,21)13-11-16-10-12-18(3,4)17-9-8-15(2)14-20(16,17)6/h7,1
InchiKey: XQCCGGBPVSNHMQ-CLPROHDKSA-N
Formula: C20H34O
SMILES: C=CC(C)(O)CCC1CCC(C)(C)C2CCC(=C)CC12C
Mol. weight [g/mol]: 290.48

Physical Properties

Property code	Value	Unit	Source
gf	171.16	kJ/mol	Joback Method
hf	-296.68	kJ/mol	Joback Method
hfus	19.21	kJ/mol	Joback Method
hvap	72.58	kJ/mol	Joback Method
log10ws	-6.10		Crippen Method
logp	5.502		Crippen Method
mcvol	268.210	ml/mol	McGowan Method
pc	1499.99	kPa	Joback Method
rinpol	1961.00		NIST Webbook
rinpol	1958.00		NIST Webbook
rinpol	1970.00		NIST Webbook
rinpol	1944.00		NIST Webbook
rinpol	1961.00		NIST Webbook
rinpol	1961.00		NIST Webbook
rinpol	1960.00		NIST Webbook
rinpol	1967.00		NIST Webbook
rinpol	1961.00		NIST Webbook
rinpol	1961.00		NIST Webbook
tb	763.49	K	Joback Method
tc	971.09	K	Joback Method
tf	451.44	K	Joback Method
vc	1.004	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	857.58	J/mol×K	763.49	Joback Method
cpg	879.64	J/mol×K	798.09	Joback Method
cpg	901.18	J/mol×K	832.69	Joback Method
cpg	922.44	J/mol×K	867.29	Joback Method
cpg	943.64	J/mol×K	901.89	Joback Method
cpg	965.01	J/mol×K	936.49	Joback Method
cpg	986.78	J/mol×K	971.09	Joback Method

Sources

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=R293293&Units=SI
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

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

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