

Manool oxide

Inchi:

InchiKey:

Formula:

SMILES:

Mol. weight [g/mol]:

InChI=1S/C20H34O/c1-7-18(4)13-9-16-19(5)12-8-11-17(2,3)15(19)10-14-20(16,6)21-18/

IGGWKHQYMAJOHK-VIHFOQNISA-N

C20H34O

C=CC1(C)CCC2C(C)(CCC3C(C)(C)CCCC32C)O1

290.48

Physical Properties

Property code	Value	Unit	Source
gf	195.90	kJ/mol	Joback Method
hf	-275.16	kJ/mol	Joback Method
hfus	16.18	kJ/mol	Joback Method
hvap	59.02	kJ/mol	Joback Method
log10ws	-6.08		Crippen Method
logp	5.743		Crippen Method
mcvol	261.650	ml/mol	McGowan Method
pc	1588.54	kPa	Joback Method
rinpol	1983.00		NIST Webbook
tb	709.15	K	Joback Method
tc	951.08	K	Joback Method
tf	459.07	K	Joback Method
vc	0.978	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	821.83	J/mol×K	709.15	Joback Method
cpg	849.99	J/mol×K	749.47	Joback Method
cpg	877.78	J/mol×K	789.79	Joback Method
cpg	905.79	J/mol×K	830.12	Joback Method
cpg	934.61	J/mol×K	870.44	Joback Method
cpg	964.82	J/mol×K	910.76	Joback Method
cpg	997.01	J/mol×K	951.08	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R613984&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
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
rinpola:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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