

1H-Naphtho[2,1-b]pyran, 3-ethenyldodecahydro-3,4a,7,7,10a-pentamethyl-, [3R-(3«alpha»,4a«beta»,6a«alpha»,10a«beta»,10b

Other names: Labd-14-ene, 8,13-epoxy-, (17R) Manoyl oxide
8«alpha»,13-Epoxyabd-14-ene
Manool oxide

Inchi: 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/

InchiKey: IGGWKHQYMAJOHK-DBYSVDLZSA-N

Formula: C20H34O

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

Mol. weight [g/mol]: 290.48

CAS: 596-84-9

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	1990.00		NIST Webbook
rinpol	1989.00		NIST Webbook
rinpol	1989.00		NIST Webbook
rinpol	1994.00		NIST Webbook
rinpol	1992.00		NIST Webbook
rinpol	1989.00		NIST Webbook
rinpol	1996.00		NIST Webbook
rinpol	1998.00		NIST Webbook
rinpol	2007.00		NIST Webbook
rinpol	1985.00		NIST Webbook
rinpol	1979.00		NIST Webbook
rinpol	1990.00		NIST Webbook
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rinpol	2000.00	NIST Webbook
rinpol	1990.00	NIST Webbook
ripol	2346.00	NIST Webbook
ripol	2339.00	NIST Webbook
ripol	2358.00	NIST Webbook
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ripol	2348.00	NIST Webbook
ripol	2347.00	NIST Webbook

ripol	2376.00		NIST Webbook
ripol	2335.00		NIST Webbook
ripol	2340.00		NIST Webbook
ripol	2345.00		NIST Webbook
tb	709.15	K	Joback Method
tc	951.08	K	Joback Method
tf	459.07	K	Joback Method
vc	0.978	m ³ /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

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=C596849&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071

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
ripol:	Polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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