

Linestrenol

Other names:	lynestrenol
Inchi:	InChI=1S/C20H28O/c1-3-20(21)13-11-18-17-9-8-14-6-4-5-7-15(14)16(17)10-12-19(18,20)
InchiKey:	YNVGQYHLRCDXFQ-UEDNIHKISA-N
Formula:	C20H28O
SMILES:	C#CC1(O)CCC2C3CCC4=CCCCC4C3CCC21C
Mol. weight [g/mol]:	284.44
CAS:	52-76-6

Physical Properties

Property code	Value	Unit	Source
gf	380.20	kJ/mol	Joback Method
hf	-19.95	kJ/mol	Joback Method
hfus	27.04	kJ/mol	Joback Method
hvap	75.20	kJ/mol	Joback Method
log10ws	-5.59		Crippen Method
logp	4.313		Crippen Method
mcvol	242.190	ml/mol	McGowan Method
pc	2051.17	kPa	Joback Method
rinpol	2319.00		NIST Webbook
rinpol	2319.00		NIST Webbook
tb	782.89	K	Joback Method
tc	1018.79	K	Joback Method
tf	529.71	K	Joback Method
vc	0.904	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	802.93	J/mol×K	782.89	Joback Method
cpg	826.27	J/mol×K	822.21	Joback Method
cpg	849.31	J/mol×K	861.52	Joback Method
cpg	872.44	J/mol×K	900.84	Joback Method
cpg	896.02	J/mol×K	940.16	Joback Method
cpg	920.43	J/mol×K	979.47	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=C52766&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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