Lup-20(29)-en-3-one

Other names: Lup-20(30)-en-3-one
Lupenone
Lupen-3-one
Inchi: InChI=1S/C30H48O/c1-19(2)20-11-14-27(5)17-18-29(7)21(25(20)27)9-10-23-28(6)15-13
InchiKey: GRBHNQFQFHLCHO-UHFFFAOYSA-N
Formula: C30H48O
SMILES: C=C(C)C1CCC2(C)CCC3(C)C(CCC4C5(C)CCC(=O)C(C)(C)C5CCC43C)C12
Mol. weight [g/mol]: 424.70
CAS: 1617-70-5

Physical Properties

Property code	Value	Unit	Source
gf	323.57	kJ/mol	Joback Method
hf	-383.05	kJ/mol	Joback Method
hfus	22.32	kJ/mol	Joback Method
hvap	79.33	kJ/mol	Joback Method
log10ws	-8.57		Crippen Method
logp	8.233		Crippen Method
mcvol	376.530	ml/mol	McGowan Method
pc	1003.98	kPa	Joback Method
rinpol	3384.20		NIST Webbook
rinpol	3384.20		NIST Webbook
tb	987.35	K	Joback Method
tc	1243.22	K	Joback Method
tf	647.24	K	Joback Method
vc	1.427	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1501.11	J/mol×K	987.35	Joback Method
cpg	1555.23	J/mol×K	1030.00	Joback Method
cpg	1614.18	J/mol×K	1072.64	Joback Method
cpg	1678.86	J/mol×K	1115.29	Joback Method

cpg	1750.16	J/mol×K	1157.93	Joback Method
cpg	1828.98	J/mol×K	1200.58	Joback Method
cpg	1916.19	J/mol×K	1243.22	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=C1617705&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