

Podocarp-7-en-3-one, 13«beta»-methyl-13-vinyl-

Other names:

Pimara-7,15-dien-3-one

Isopimara-7,15-dien-3-one

Inchi: InChI=1S/C20H30O/c1-6-19(4)11-9-15-14(13-19)7-8-16-18(2,3)17(21)10-12-20(15,16)5/

InchiKey: YAXFLCDQLAZOPS-UHFFFAOYSA-N

Formula: C20H30O

SMILES: C=CC1(C)CCC2C(=CCC3C(C)(C)C(=O)CCC23C)C1

Mol. weight [g/mol]: 286.45

CAS: 7715-48-2

Physical Properties

Property code	Value	Unit	Source
gf	192.96	kJ/mol	Joback Method
hf	-229.45	kJ/mol	Joback Method
hfus	13.77	kJ/mol	Joback Method
hvap	61.17	kJ/mol	Joback Method
log10ws	-5.66		Crippen Method
logp	5.321		Crippen Method
mcvol	253.050	ml/mol	McGowan Method
pc	1657.84	kPa	Joback Method
rinpol	2279.00		NIST Webbook
rinpol	2227.00		NIST Webbook
tb	758.59	K	Joback Method
tc	1008.37	K	Joback Method
tf	494.34	K	Joback Method
vc	0.953	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	807.74	J/molxK	758.59	Joback Method
cpg	834.81	J/molxK	800.22	Joback Method
cpg	861.72	J/molxK	841.85	Joback Method
cpg	888.95	J/molxK	883.48	Joback Method
cpg	916.96	J/molxK	925.11	Joback Method

cpg	946.23	J/mol×K	966.74	Joback Method
cpg	977.24	J/mol×K	1008.37	Joback Method

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
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=C7715482&Units=SI

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
hvac:	Enthalpy of vaporization at standard conditions
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mccvol:	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

Latest version available from:

<https://www.chemeo.com/cid/44-654-7/Podocarp-7-en-3-one-13-beta-methyl-13-vinyl.pdf>

Generated by Cheméo on 2024-04-20 03:33:39.118567617 +0000 UTC m=+15873268.039144933.

Cheméo (<https://www.chemeo.com>) is the biggest free database of chemical and physical data for the process industry.