Isopimara-7,15-dien-3-one

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/h
InchiKey: YAXFLCDQLAZOPS-UHFFFAOYSA-N
Formula: C20H30O
SMILES: C=CC1(C)CCC2C(=CCC3C(C)(C)C(=O)CCC23C)C1
Mol. weight [g/mol]: 286.46

Physical Properties

Property code	Value	Unit	Source
hfus	13.77	kJ/mol	Joback Method
logp	5.321		Crippen Method
mcvol	253.050	ml/mol	McGowan Method
rinpol	2227.00		NIST Webbook
rinpol	2279.00		NIST Webbook
rinpol	2227.00		NIST Webbook

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	807.74	J/mol×K	758.59	Joback Method
cpg	834.81	J/mol×K	800.22	Joback Method
cpg	861.72	J/mol×K	841.85	Joback Method
cpg	888.95	J/mol×K	883.48	Joback Method
cpg	916.96	J/mol×K	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/ci990307l

Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Cheméo Relay (1.0):	
Cheméo Relay (1.0, beta):	
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C7715482&Units=SI
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

Legend

cpg:	Ideal gas heat capacity
hfus:	Enthalpy of fusion at standard conditions
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
rinpol:	Non-polar retention indices