

Isopimarane

Inchi:	InChI=1S/C20H36/c1-6-19(4)13-10-16-15(14-19)8-9-17-18(2,3)11-7-12-20(16,17)5/h15-1
InchiKey:	GZHFBZCDMVGRTI-GTSVPISWSA-N
Formula:	C20H36
SMILES:	CCC1(C)CCC2C(CCC3C(C)(C)CCCC23C)C1
Mol. weight [g/mol]:	276.50

Physical Properties

Property code	Value	Unit	Source
gf	199.67	kJ/mol	Joback Method
hf	-283.83	kJ/mol	Joback Method
hfus	15.78	kJ/mol	Joback Method
hvap	56.33	kJ/mol	Joback Method
log10ws	-6.43		Crippen Method
logp	6.445		Crippen Method
mcvol	260.080	ml/mol	McGowan Method
pc	1494.19	kPa	Joback Method
rinpol	1950.00		NIST Webbook
rinpol	2019.00		NIST Webbook
rinpol	2019.00		NIST Webbook
tb	685.28	K	Joback Method
tc	917.18	K	Joback Method
tf	410.36	K	Joback Method
vc	0.978	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	811.77	J/molxK	685.28	Joback Method
cpg	840.70	J/molxK	723.93	Joback Method
cpg	868.58	J/molxK	762.58	Joback Method
cpg	895.82	J/molxK	801.23	Joback Method
cpg	922.83	J/molxK	839.88	Joback Method
cpg	950.02	J/molxK	878.53	Joback Method
cpg	977.79	J/molxK	917.18	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R312493&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.cheméo.com/doc/models/crippen_log10ws
Joback Method:	https://en.wikipedia.org/wiki/Joback_method

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
h vap:	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
r in pol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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