pimarinol

Inchi: InChI=1S/C20H32O/c1-5-18(2)12-9-16-15(13-18)7-8-17-19(3,14-21)10-6-11-20(16,17)4/h5,15-17,21H,1-2,6-14H2,3-4H3/t15-,16+,17+,18+,19+,20+/m1/s1
InchiKey: JEOZUAHPKAVXSF-OBKDMQGPSA-N
Formula: C20H32O
SMILES: C=CC1(C)C=C2CCC3C(C)(CO)CCCC3(C)C2CC1
Mol. weight [g/mol]: 288.47

Physical Properties

Property code	Value	Unit	Source
gf	178.73	kJ/mol	Joback Method
hf	-243.98	kJ/mol	Joback Method
hfus	18.35	kJ/mol	Joback Method
hvap	73.61	kJ/mol	Joback Method
log10ws	-5.64		Crippen Method
logp	5.114		Crippen Method
mcvol	257.350	ml/mol	McGowan Method
pc	1737.56	kPa	Joback Method
rinpol	2226.00		NIST Webbook
rinpol	2226.00		NIST Webbook
rinpol	2240.00		NIST Webbook
tb	782.95	K	Joback Method
tc	1004.60	K	Joback Method
tf	486.94	K	Joback Method
vc	0.965	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	841.59	J/mol×K	782.95	Joback Method
cpg	865.45	J/mol×K	819.89	Joback Method
cpg	889.43	J/mol×K	856.83	Joback Method
cpg	913.91	J/mol×K	893.78	Joback Method
cpg	939.25	J/mol×K	930.72	Joback Method
cpg	965.82	J/mol×K	967.66	Joback Method
cpg	993.99	J/mol×K	1004.60	Joback Method

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
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=R167278&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
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