Isopimara-8,15-diene

Other names: 8,15-Isopimaradiene
Inchi: InChI=1S/C20H32/c1-6-19(4)13-10-16-15(14-19)8-9-17-18(2,3)11-7-12-20(16,17)5/h6,17
InchiKey: OROJBMPJDLLRFD-MFUMQWNRSA-N
Formula: C20H32
SMILES: C=CC1(C)CCC2=C(CCC3C(C)(C)CCCC23C)C1
Mol. weight [g/mol]: 272.47

Physical Properties

Property code	Value	Unit	Source
gf	313.63	kJ/mol	Joback Method
hf	-82.88	kJ/mol	Joback Method
hfus	12.80	kJ/mol	Joback Method
hvap	57.90	kJ/mol	Joback Method
log10ws	-6.62		Crippen Method
logp	6.286		Crippen Method
mcvol	251.480	ml/mol	McGowan Method
pc	1635.13	kPa	Joback Method
rinpol	1906.00		NIST Webbook
rinpol	1921.00		NIST Webbook
rinpol	1908.00		NIST Webbook
rinpol	1906.00		NIST Webbook
rinpol	1915.00		NIST Webbook
rinpol	1898.00		NIST Webbook
ripol	2175.00		NIST Webbook
ripol	2165.00		NIST Webbook
ripol	2175.00		NIST Webbook
ripol	2210.00		NIST Webbook
tb	700.42	K	Joback Method
tc	940.52	K	Joback Method
tf	442.88	K	Joback Method
vc	0.947	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	761.41	J/mol×K	700.42	Joback Method
cpg	787.70	J/mol×K	740.44	Joback Method
cpg	813.29	J/mol×K	780.45	Joback Method
cpg	838.65	J/mol×K	820.47	Joback Method
cpg	864.25	J/mol×K	860.49	Joback Method
cpg	890.55	J/mol×K	900.51	Joback Method
cpg	918.02	J/mol×K	940.52	Joback Method

Sources

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=R27338&Units=SI
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws

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
ripol: Polar retention indices
tb: Normal Boiling Point Temperature
tc: Critical Temperature
tf: Normal melting (fusion) point
vc: Critical Volume

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