

Isopatchoula-3,5-diene

Inchi:	InChI=1S/C15H22/c1-10-7-8-15-11(2)5-6-12(9-13(10)15)14(15,3)4/h5-6,9-11,13H,7-8H2
InchiKey:	OCEGSQBSJHCVPS-NYXKVOKKSA-N
Formula:	C15H22
SMILES:	CC1CCC23C(C)C=CC(=CC12)C3(C)C
Mol. weight [g/mol]:	202.34

Physical Properties

Property code	Value	Unit	Source
gf	257.36	kJ/mol	Joback Method
hf	-52.96	kJ/mol	Joback Method
hfus	16.41	kJ/mol	Joback Method
hvap	47.39	kJ/mol	Joback Method
log10ws	-4.28		Crippen Method
logp	4.191		Crippen Method
mcvol	181.030	ml/mol	McGowan Method
pc	2189.73	kPa	Joback Method
rinpol	1392.00		NIST Webbook
rinpol	1374.00		NIST Webbook
rinpol	1392.00		NIST Webbook
rinpol	1374.00		NIST Webbook
ripol	1553.00		NIST Webbook
ripol	1553.00		NIST Webbook
ripol	1541.00		NIST Webbook
tb	565.80	K	Joback Method
tc	793.56	K	Joback Method
tf	358.95	K	Joback Method
vc	0.697	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	483.94	J/mol×K	565.80	Joback Method
cpg	505.80	J/mol×K	603.76	Joback Method
cpg	526.11	J/mol×K	641.72	Joback Method

cpg	545.16	J/mol×K	679.68	Joback Method
cpg	563.26	J/mol×K	717.64	Joback Method
cpg	580.73	J/mol×K	755.60	Joback Method
cpg	597.85	J/mol×K	793.56	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R411862&Units=SI
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

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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