

Trichodiene

Inchi: InChI=1S/C15H24/c1-12-7-10-14(3,11-8-12)15(4)9-5-6-13(15)2/h7H,2,5-6,8-11H2,1,3-4H
InchiKey: YFLSTROSSKYYNK-LSDHHAUSA-N
Formula: C15H24
SMILES: C=C1CCCC1(C)C1(C)CC=C(C)CC1
Mol. weight [g/mol]: 204.35

Physical Properties

Property code	Value	Unit	Source
gf	198.85	kJ/mol	Joback Method
hf	-77.10	kJ/mol	Joback Method
hfus	7.45	kJ/mol	Joback Method
hvap	48.48	kJ/mol	Joback Method
log10ws	-5.11		Crippen Method
logp	4.869		Crippen Method
mcvol	191.890	ml/mol	McGowan Method
pc	2177.49	kPa	Joback Method
rinpol	1541.00		NIST Webbook
rinpol	1541.00		NIST Webbook
rinpol	1533.00		NIST Webbook
tb	581.21	K	Joback Method
tc	816.28	K	Joback Method
tf	351.85	K	Joback Method
vc	0.716	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	499.46	J/molxK	581.21	Joback Method
cpg	522.35	J/molxK	620.39	Joback Method
cpg	543.78	J/molxK	659.57	Joback Method
cpg	564.03	J/molxK	698.74	Joback Method
cpg	583.37	J/molxK	737.92	Joback Method
cpg	602.08	J/molxK	777.10	Joback Method
cpg	620.44	J/molxK	816.28	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R292750&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
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

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
hvp:	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
rinp:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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