

Isodaucadiene

Inchi:	InChI=1S/C15H26/c1-11(2)13-7-9-15(4)8-5-6-12(3)10-14(13)15/h11,13-14H,3,5-10H2,1-
InchiKey:	XXJBDHLFOFXLLR-RBSFLKMASA-N
Formula:	C15H26
SMILES:	<chem>C=C1CCCC2(C)CCC(C(C)C)C2C1</chem>
Mol. weight [g/mol]:	206.37

Physical Properties

Property code	Value	Unit	Source
gf	185.96	kJ/mol	Joback Method
hf	-158.11	kJ/mol	Joback Method
hfus	12.57	kJ/mol	Joback Method
hvap	47.81	kJ/mol	Joback Method
log10ws	-4.78		Crippen Method
logp	4.805		Crippen Method
mcvol	196.190	ml/mol	McGowan Method
pc	1959.60	kPa	Joback Method
rinsol	1383.00		NIST Webbook
tb	567.45	K	Joback Method
tc	787.08	K	Joback Method
tf	298.95	K	Joback Method
vc	0.733	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	519.21	J/mol×K	567.45	Joback Method
cpg	543.58	J/mol×K	604.06	Joback Method
cpg	566.48	J/mol×K	640.66	Joback Method
cpg	588.03	J/mol×K	677.27	Joback Method
cpg	608.38	J/mol×K	713.87	Joback Method
cpg	627.68	J/mol×K	750.48	Joback Method
cpg	646.08	J/mol×K	787.08	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R571607&Units=SI
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

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

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