

(E,E)-1,6-Cyclodecadiene, 3-methyl

Inchi:	InChI=1S/C13H22/c1-13-11-9-7-5-3-2-4-6-8-10-12-13/h5,7,10,12-13H,2-4,6,8-9,11H2,1H
InchiKey:	XSGFFXSJYTYKAO-WRRYRWARSA-N
Formula:	C13H22
SMILES:	CC1C=CCCCCCC=CCC1
Mol. weight [g/mol]:	178.31

Physical Properties

Property code	Value	Unit	Source
gf	70.35	kJ/mol	Joback Method
hf	-178.73	kJ/mol	Joback Method
hfus	11.10	kJ/mol	Joback Method
hvap	46.58	kJ/mol	Joback Method
log10ws	-4.62		Crippen Method
logp	4.479		Crippen Method
mvol	174.570	ml/mol	McGowan Method
pc	2405.28	kPa	Joback Method
rinpol	1135.00		NIST Webbook
tb	540.33	K	Joback Method
tc	780.92	K	Joback Method
tf	224.05	K	Joback Method
vc	0.621	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	416.72	J/mol×K	540.33	Joback Method
cpg	443.11	J/mol×K	580.43	Joback Method
cpg	467.93	J/mol×K	620.53	Joback Method
cpg	491.15	J/mol×K	660.62	Joback Method
cpg	512.79	J/mol×K	700.72	Joback Method
cpg	532.81	J/mol×K	740.82	Joback Method
cpg	551.23	J/mol×K	780.92	Joback Method
dvisc	0.0729791	Paxs	224.05	Joback Method
dvisc	0.0070607	Paxs	276.76	Joback Method

dvisc	0.0014424	Paxs	329.48	Joback Method
dvisc	0.0004566	Paxs	382.19	Joback Method
dvisc	0.0001911	Paxs	434.90	Joback Method
dvisc	0.0000965	Paxs	487.62	Joback Method
dvisc	0.0000557	Paxs	540.33	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=R2736&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
dvisc:	Dynamic viscosity
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

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