

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

Inchi:	InChI=1S/C13H22/c1-13-11-9-7-5-3-2-4-6-8-10-12-13/h2-3,11H,4-10,12H2,1H3/b3-2+,13
InchiKey:	QYOLEDPEVIWBHX-SXBUOHTDSA-N
Formula:	C13H22
SMILES:	CC1=CCCCC=CCCCC1
Mol. weight [g/mol]:	178.31

Physical Properties

Property code	Value	Unit	Source
gf	68.43	kJ/mol	Joback Method
hf	-169.86	kJ/mol	Joback Method
hfus	9.64	kJ/mol	Joback Method
hvap	47.55	kJ/mol	Joback Method
log10ws	-4.87		Crippen Method
logp	4.623		Crippen Method
mvol	174.570	ml/mol	McGowan Method
pc	2448.32	kPa	Joback Method
rinpol	1178.00		NIST Webbook
tb	549.98	K	Joback Method
tc	791.73	K	Joback Method
tf	240.81	K	Joback Method
vc	0.622	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	417.50	J/molxK	549.98	Joback Method
cpg	529.38	J/molxK	751.44	Joback Method
cpg	510.11	J/molxK	711.15	Joback Method
cpg	489.28	J/molxK	670.86	Joback Method
cpg	466.90	J/molxK	630.56	Joback Method
cpg	442.97	J/molxK	590.27	Joback Method
cpg	547.09	J/molxK	791.73	Joback Method
dvisc	0.0000471	Paxs	549.98	Joback Method
dvisc	0.0000820	Paxs	498.45	Joback Method

dvisc	0.0001619	Paxs	446.92	Joback Method
dvisc	0.0003821	Paxs	395.39	Joback Method
dvisc	0.0011660	Paxs	343.87	Joback Method
dvisc	0.0052729	Paxs	292.34	Joback Method
dvisc	0.0454859	Paxs	240.81	Joback Method

Sources

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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R2723&Units=SI

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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