

(E)-Cyclododecene, 1-methyl

Other names:	trans-Cyclododecene, 1-methyl-
Inchi:	InChI=1S/C13H24/c1-13-11-9-7-5-3-2-4-6-8-10-12-13/h11H,2-10,12H2,1H3/b13-11+
InchiKey:	YWYIHWJAVXCTFB-ACCUITESSA-N
Formula:	C13H24
SMILES:	CC1=CCCCCCCCCCC1
Mol. weight [g/mol]:	180.33

Physical Properties

Property code	Value	Unit	Source
gf	38.47	kJ/mol	Joback Method
hf	-227.64	kJ/mol	Joback Method
hfus	8.42	kJ/mol	Joback Method
hvap	47.26	kJ/mol	Joback Method
log10ws	-5.01		Crippen Method
logp	4.847		Crippen Method
mcvol	178.870	ml/mol	McGowan Method
pc	2363.37	kPa	Joback Method
rinpol	1382.00		NIST Webbook
rinpol	1382.00		NIST Webbook
rinpol	1382.00		NIST Webbook
tb	550.82	K	Joback Method
tc	790.09	K	Joback Method
tf	240.05	K	Joback Method
vc	0.635	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	436.55	J/molxK	550.82	Joback Method
cpg	554.12	J/molxK	750.21	Joback Method
cpg	533.78	J/molxK	710.33	Joback Method
cpg	511.85	J/molxK	670.46	Joback Method
cpg	488.33	J/molxK	630.58	Joback Method
cpg	463.22	J/molxK	590.70	Joback Method

cpg	572.86	J/mol×K	790.09	Joback Method
dvisc	0.0000464	Paxs	550.82	Joback Method
dvisc	0.0000823	Paxs	499.02	Joback Method
dvisc	0.0001667	Paxs	447.23	Joback Method
dvisc	0.0004060	Paxs	395.43	Joback Method
dvisc	0.0012932	Paxs	343.64	Joback Method
dvisc	0.0062150	Paxs	291.85	Joback Method
dvisc	0.0588073	Paxs	240.05	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R2621&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
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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