

Cyclododecene, (E)-

Other names:	(E)-Cyclododecene trans-Cyclododecene Cyclododecene, trans- t-Cyclododecene
Inchi:	InChI=1S/C12H22/c1-2-4-6-8-10-12-11-9-7-5-3-1/h1-2H,3-12H2/b2-1+
InchiKey:	HYPABJGVBDSCIT-OWOJBTEDSA-N
Formula:	C12H22
SMILES:	C1=CCCCCCCCCCC1
Mol. weight [g/mol]:	166.30
CAS:	1486-75-5

Physical Properties

Property code	Value	Unit	Source
gf	39.68	kJ/mol	Joback Method
hf	-195.53	kJ/mol	Joback Method
hfus	6.22	kJ/mol	Joback Method
hvap	44.37	kJ/mol	Joback Method
ie	8.74 ± 0.15	eV	NIST Webbook
log10ws	-4.59		Crippen Method
logp	4.457		Crippen Method
mcvol	164.780	ml/mol	McGowan Method
pc	2640.67	kPa	Joback Method
rinpol	1342.00		NIST Webbook
rinpol	1291.50		NIST Webbook
rinpol	1336.70		NIST Webbook
rinpol	1306.00		NIST Webbook
rinpol	1306.00		NIST Webbook
rinpol	1306.00		NIST Webbook
rinpol	1362.00		NIST Webbook
rinpol	1356.00		NIST Webbook
rinpol	1342.00		NIST Webbook
rinpol	1336.70		NIST Webbook
rinpol	1354.00		NIST Webbook
rinpol	1344.00		NIST Webbook
rinpol	1356.00		NIST Webbook
rinpol	1306.00		NIST Webbook
rinpol	1306.00		NIST Webbook

ripol	1539.80		NIST Webbook
ripol	1557.90		NIST Webbook
ripol	1577.90		NIST Webbook
tb	522.96	K	Joback Method
tc	765.93	K	Joback Method
tf	216.26	K	Joback Method
vc	0.580	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	383.42	J/mol×K	522.96	Joback Method
cpg	410.08	J/mol×K	563.46	Joback Method
cpg	435.15	J/mol×K	603.95	Joback Method
cpg	458.64	J/mol×K	644.45	Joback Method
cpg	480.53	J/mol×K	684.94	Joback Method
cpg	500.83	J/mol×K	725.44	Joback Method
cpg	519.53	J/mol×K	765.93	Joback Method
dvisc	0.1989191	Pa×s	216.26	Joback Method
dvisc	0.0140649	Pa×s	267.38	Joback Method
dvisc	0.0023276	Pa×s	318.49	Joback Method
dvisc	0.0006335	Pa×s	369.61	Joback Method
dvisc	0.0002366	Pa×s	420.73	Joback Method
dvisc	0.0001094	Pa×s	471.84	Joback Method
dvisc	0.0000588	Pa×s	522.96	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C1486755&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
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
ie:	Ionization energy
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
ripol:	Polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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