

1,5-Cyclododecadiene, (e,e)-

Other names:	trans,trans-1,5-Cyclododecadiene 1,5-Cyclododecadiene, trans,trans- t,t-Cyclododeca-1,5-diene
Inchi:	InChI=1S/C12H20/c1-2-4-6-8-10-12-11-9-7-5-3-1/h1-2,7,9H,3-6,8,10-12H2/b2-1-,9-7?
InchiKey:	KEMUGHMYINTXKW-ATTBXNPTSA-N
Formula:	C12H20
SMILES:	C1=C/CCCCC/C=C/CC/1
Mol. weight [g/mol]:	164.29

Physical Properties

Property code	Value	Unit	Source
af	0.1786		Cheméo Relay (1.0)
gf	69.64	kJ/mol	Joback Method
hf	3.54	kJ/mol	Cheméo Relay (1.0)
hfus	7.44	kJ/mol	Joback Method
hvap	58.80	kJ/mol	Cheméo Relay (1.0)
ie	8.50	eV	Cheméo Relay (1.0)
log10ws	-4.48		Cheméo Relay (1.0)
logp	4.233		Crippen Method
mcvol	160.480	ml/mol	McGowan Method
pc	2741.15	kPa	Joback Method
rinpol	1341.00		NIST Webbook
rinpol	1332.00		NIST Webbook
rinpol	1321.00		NIST Webbook
tb	509.38	K	Cheméo Relay (1.0)
tc	692.68	K	Cheméo Relay (1.0)
tf	250.02	K	Cheméo Relay (1.0)
vc	0.518	m3/kmol	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	365.45	J/mol×K	522.12	Joback Method
cpg	390.85	J/mol×K	563.05	Joback Method

cpg	414.69	J/mol×K	603.97	Joback Method
cpg	436.97	J/mol×K	644.90	Joback Method
cpg	457.70	J/mol×K	685.83	Joback Method
cpg	476.87	J/mol×K	726.75	Joback Method
cpg	494.48	J/mol×K	767.68	Joback Method
dvisc	0.1459004	Pa×s	217.02	Joback Method
dvisc	0.0115346	Pa×s	267.87	Joback Method
dvisc	0.0020493	Pa×s	318.72	Joback Method
dvisc	0.0005857	Pa×s	369.57	Joback Method
dvisc	0.0002267	Pa×s	420.42	Joback Method
dvisc	0.0001077	Pa×s	471.27	Joback Method
dvisc	0.0000591	Pa×s	522.12	Joback Method

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Cheméo Relay (1.0):	
Cheméo Relay (1.0, beta):	
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C1684055&Units=SI
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

Legend

af:	Acentric Factor
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

tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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