1,5,9-Cyclododecatriene, (E,E,Z)-

Other names:	cis-1, trans-5, trans-9-Cyclododecatriene
	cis,trans,trans-1,5,9-Cyclododecatriene
	trans-trans-cis-1,5,9-Cyclodecatriene
	trans,trans,cis-1,5,9-Cyclododecatriene
	(E,E,Z)-1,5,9-Cyclododecatriene
	(1E,5E,9Z)-Cyclododeca-1,5,9-triene
	1,5,9-Cyclododecatriene, (1E,5E,9Z)-
Inchi:	InChI=1S/C12H18/c1-2-4-6-8-10-12-11-9-7-5-3-1/h1-2,7-10H,3-6,11-12H2/b2-1-,9-7+,10
InchiKey:	ZOLLIQAKMYWTBR-RYMQXAEESA-N
Formula:	C12H18
SMILES:	C1=CCCC=CCCC=CCC1
Mol. weight [g/mol]:	162.27
CAS:	706-31-0

Physical Properties

Property code	Value	Unit	Source
chl	-7324.50	kJ/mol	NIST Webbook
gf	99.60	kJ/mol	Joback Method
hf	-79.97	kJ/mol	Joback Method
hfus	8.67	kJ/mol	Joback Method
hvap	67.20	kJ/mol	NIST Webbook
log10ws	-4.30		Crippen Method
logp	4.009		Crippen Method
mcvol	156.180	ml/mol	McGowan Method
pc	2847.48	kPa	Joback Method
rinpol	1329.00		NIST Webbook
rinpol	1338.00		NIST Webbook
rinpol	1284.00		NIST Webbook
rinpol	1292.00		NIST Webbook
rinpol	1296.00		NIST Webbook
rinpol	1284.00		NIST Webbook
rinpol	1279.00		NIST Webbook
rinpol	1329.00		NIST Webbook
rinpol	1346.00		NIST Webbook
tb	521.28	K	Joback Method
tc	769.47	K	Joback Method
tf	217.78	K	Joback Method

vc	0.551	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	347.56	J/mol×K	521.28	Joback Method
cpg	469.35	J/mol×K	769.47	Joback Method
cpg	452.85	J/mol×K	728.10	Joback Method
cpg	434.83	J/mol×K	686.74	Joback Method
cpg	415.29	J/mol×K	645.37	Joback Method
cpg	394.23	J/mol×K	604.01	Joback Method
cpg	371.65	J/mol×K	562.64	Joback Method
cpl	287.76	J/mol×K	298.15	NIST Webbook
dvisc	0.0094713	Pa×s	268.36	Joback Method
dvisc	0.0000594	Pa×s	521.28	Joback Method
dvisc	0.0001059	Pa×s	470.70	Joback Method
dvisc	0.0002171	Pa×s	420.11	Joback Method
dvisc	0.0005414	Pa×s	369.53	Joback Method
dvisc	0.0018048	Pa×s	318.95	Joback Method
dvisc	0.1073633	Pa×s	217.78	Joback Method
hvapt	68.00	kJ/mol	329.50	NIST Webbook

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=C706310&Units=SI
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws

Legend

chl: Standard liquid enthalpy of combustion
cpg: Ideal gas heat capacity
cpl: Liquid phase 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
hvapt:	Enthalpy of vaporization at a given temperature
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