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

Other names:	(E,E,E)-1,5,9-Cyclododecatriene
	All-trans-1,5,9-Cyclododecatriene
	trans,trans,trans-1,5,9-Cyclododecatriene
	(1E,5E,9E)-cyclododeca-1,5,9-triene
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-FFWAUJBHSA-N
Formula:	C12H18
SMILES:	C1=CCCC=CCCC=CCC1
Mol. weight [g/mol]:	162.27
CAS:	676-22-2

Physical Properties

Property code	Value	Unit	Source
chs	-7321.20	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
hsub	74.68	kJ/mol	NIST Webbook
hvap	44.95	kJ/mol	Joback Method
log10ws	-4.30		Crippen Method
logp	4.009		Crippen Method
mcvol	156.180	ml/mol	McGowan Method
pc	2847.48	kPa	Joback Method
rinpol	1264.00		NIST Webbook
rinpol	1256.00		NIST Webbook
rinpol	1260.00		NIST Webbook
rinpol	1269.00		NIST Webbook
rinpol	1312.00		NIST Webbook
rinpol	1303.00		NIST Webbook
tb	510.70	K	NIST Webbook
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	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
cpg	347.56	J/mol×K	521.28	Joback Method
dvisc	0.1073633	Pa×s	217.78	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	0.0094713	Pa×s	268.36	Joback Method
hsubt	75.20	kJ/mol	290.00	NIST Webbook

Sources

McGowan Method: http://link.springer.com/article/10.1007/BF02311772
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C676222&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

Legend

chs: Standard solid enthalpy of combustion
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
hsub: Enthalpy of sublimation at standard conditions

hsubt:	Enthalpy of sublimation at a given temperature
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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