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

Other names:	1,5,9-Cyclododecatriene, cis,cis,cis- cis,cis,cis-1,5,9-Cyclododecatriene
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-MOLCZBCNSA-N
Formula:	C12H18
SMILES:	C1=CCCC=CCCC=CCC1
Mol. weight [g/mol]:	162.27
CAS:	4736-48-5

Physical Properties

Property code	Value	Unit	Source
gf	99.60	kJ/mol	Joback Method
hf	-79.97	kJ/mol	Joback Method
hfus	8.67	kJ/mol	Joback Method
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	1294.00		NIST Webbook
rinpol	1290.00		NIST Webbook
rinpol	1294.00		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	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	469.35	J/mol×K	769.47	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
dvisc	0.1073633	Pa×s	217.78	Joback Method

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.09261e+01
Coeff. B	-2.76954e+03
Coeff. C	-7.50810e+01
Temperature range (K), min.	335.41
Temperature range (K), max.	568.35

Sources

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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C4736485&Units=SI
The Yaws Handbook of Vapor Pressure:	https://www.sciencedirect.com/book/9780128029992/the-yaws-handbook-of-vapor-pressure

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
pvap:	Vapor 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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