

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	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	347.56	J/molxK	521.28	Joback Method
cpg	452.85	J/molxK	728.10	Joback Method
cpg	434.83	J/molxK	686.74	Joback Method
cpg	415.29	J/molxK	645.37	Joback Method

cpg	394.23	J/molxK	604.01	Joback Method
cpg	371.65	J/molxK	562.64	Joback Method
cpg	469.35	J/molxK	769.47	Joback Method
dvisc	0.0000594	Paxs	521.28	Joback Method
dvisc	0.0001059	Paxs	470.70	Joback Method
dvisc	0.0002171	Paxs	420.11	Joback Method
dvisc	0.0005414	Paxs	369.53	Joback Method
dvisc	0.0018048	Paxs	318.95	Joback Method
dvisc	0.0094713	Paxs	268.36	Joback Method
dvisc	0.1073633	Paxs	217.78	Joback Method

Correlations

Information	Value
Property code	pvap
Equation	$\ln(P_{vp}) = A + B/(T + C)$
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:	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
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307I

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
h vap:	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
r in pol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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