1,5,9-Cyclododecatriene

Other names:	1,5,9-Cyclododecatriene (Z,E,E)
	1,5,9-Cyclooctatriene
	1-cis-5-trans-9-trans-cyclododecatriene
	CDT
	Cyclododecatriene
	UN 2518
	cis,trans,trans-Cyclododeca-1,5,9-triene
	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-MOLCZBCNSA-N
Formula:	C12H18
SMILES:	C1=CCCC=CCCC=CCC1
Mol. weight [g/mol]:	162.27
CAS:	4904-61-4

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	1256.00		NIST Webbook
rinpol	1256.00		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	371.65	J/mol×K	562.64	Joback Method
cpg	394.23	J/mol×K	604.01	Joback Method
cpg	415.29	J/mol×K	645.37	Joback Method
cpg	434.83	J/mol×K	686.74	Joback Method
cpg	452.85	J/mol×K	728.10	Joback Method
cpg	469.35	J/mol×K	769.47	Joback Method
dvisc	0.0094713	Pa×s	268.36	Joback Method
dvisc	0.1073633	Pa×s	217.78	Joback Method
dvisc	0.0018048	Pa×s	318.95	Joback Method
dvisc	0.0005414	Pa×s	369.53	Joback Method
dvisc	0.0002171	Pa×s	420.11	Joback Method
dvisc	0.0001059	Pa×s	470.70	Joback Method
dvisc	0.0000594	Pa×s	521.28	Joback Method
hvapt	49.90	kJ/mol	365.50	NIST Webbook
hvapt	60.00	kJ/mol	411.50	NIST Webbook
hvapt	47.80	kJ/mol	464.50	NIST Webbook

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.25025e+01
Coeff. B	-3.38959e+03
Coeff. C	-8.42230e+01
Temperature range (K), min.	361.72
Temperature range (K), max.	555.59

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=C4904614&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
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
pvap:	Vapor pressure
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume