(Z,E,Z)-1,5,9-Cyclododecatriene, 3-methyl

Inchi: InChI=1S/C13H20/c1-13-11-9-7-5-3-2-4-6-8-10-12-13/h2-3,8-11,13H,4-7,12H2,1H3/b3-2
InchiKey: OQDOPRBIIHXPJP-CRVPFISASA-N
Formula: C13H20
SMILES: CC1C=CCCC=CCCC=CC1
Mol. weight [g/mol]: 176.30

Physical Properties

Property code	Value	Unit	Source
af	0.1871		Cheméo Relay (1.0)
hf	-23.38	kJ/mol	Cheméo Relay (1.0)
hfus	12.33	kJ/mol	Joback Method
hvap	64.95	kJ/mol	Cheméo Relay (1.0)
ie	8.33	eV	Cheméo Relay (1.0)
logp	4.255		Crippen Method
mcvol	170.270	ml/mol	McGowan Method
pc	2492.52	kPa	Joback Method
rinpol	1337.00		NIST Webbook
tb	516.51	K	Cheméo Relay (1.0)
tc	680.47	K	Cheméo Relay (1.0)
tf	232.00	K	Cheméo Relay (1.0)
vc	0.550	m3/kmol	Cheméo Relay (1.0)

Correlations

Information	Value
Property code	cpg
Equation	$Y = A + B \cdot T + C \cdot T^2 + D \cdot T^3 + E \cdot T.$
Y unit	J/mol×K
Coeff. A	-8.19200e+01
Coeff. B	1.13532e+00
Coeff. C	-4.47840e-04
Coeff. D	-1.37000e-08
Coeff. E	0.00000e+00
Basis	predicted

Temperature range (K), min.	273.00
Temperature range (K), max.	1000.00

Information	Value
Property code	dvisc
Equation	Y = exp(A + B/T + C·ln(T) + D·T^E)
Y unit	Pa×s
Coeff. A	-1.46998e+01
Coeff. B	2.65173e+03
Coeff. C	0.00000e+00
Coeff. D	0.00000e+00
Coeff. E	0.00000e+00
Basis	predicted
Comment	Liquid phase. Joback/Reid (1987), valid from Tf to 0.7·Tc.
Temperature range (K), min.	224.81
Temperature range (K), max.	548.02

Sources

Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws
Cheméo Relay (1.0):
Cheméo Relay (1.0, beta):
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=R3017&Units=SI
Joback Method: https://en.wikipedia.org/wiki/Joback_method
McGowan Method: http://link.springer.com/article/10.1007/BF02311772

Legend

af: Acentric Factor
cpg: Ideal gas heat capacity
dvisc: Dynamic viscosity
hf: Enthalpy of formation at standard conditions
hfus: Enthalpy of fusion at standard conditions
hvap: Enthalpy of vaporization at standard conditions
ie: Ionization energy
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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