

(Z,Z,E)-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:

OQDOPRBIHXJP-VWEHVJGJSA-N

Formula:

C13H20

SMILES:

CC1C=CCCC=CCCC=CC1

Mol. weight [g/mol]:

176.30

Physical Properties

Property code	Value	Unit	Source
gf	100.31	kJ/mol	Joback Method
hf	-120.95	kJ/mol	Joback Method
hfus	12.33	kJ/mol	Joback Method
hvap	46.87	kJ/mol	Joback Method
log10ws	-4.48		Crippen Method
logp	4.255		Crippen Method
mcvol	170.270	ml/mol	McGowan Method
pc	2492.52	kPa	Joback Method
rinpol	1331.00		NIST Webbook
tb	539.49	K	Joback Method
tc	782.60	K	Joback Method
tf	224.81	K	Joback Method
vc	0.607	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	398.08	J/molxK	539.49	Joback Method
cpg	423.24	J/molxK	580.01	Joback Method
cpg	446.86	J/molxK	620.53	Joback Method
cpg	468.92	J/molxK	661.04	Joback Method
cpg	489.42	J/molxK	701.56	Joback Method
cpg	508.36	J/molxK	742.08	Joback Method
cpg	525.73	J/molxK	782.60	Joback Method
dvisc	0.0547834	Paxs	224.81	Joback Method
dvisc	0.0058834	Paxs	277.26	Joback Method

dvisc	0.0012850	Paxs	329.70	Joback Method
dvisc	0.0004261	Paxs	382.15	Joback Method
dvisc	0.0001844	Paxs	434.60	Joback Method
dvisc	0.0000956	Paxs	487.04	Joback Method
dvisc	0.0000563	Paxs	539.49	Joback Method

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=R3091&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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
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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