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

Inchi: InChI=1S/C13H20/c1-13-11-9-7-5-3-2-4-6-8-10-12-13/h3,5-6,8,11H,2,4,7,9-10,12H2,1H3
InchiKey: VJHWJWRAAFGNQY-ANVYFWARSA-N
Formula: C13H20
SMILES: CC1=CCCC=CCCC=CCC1
Mol. weight [g/mol]: 176.30

Physical Properties

Property code	Value	Unit	Source
gf	98.39	kJ/mol	Joback Method
hf	-112.08	kJ/mol	Joback Method
hfus	10.87	kJ/mol	Joback Method
hvap	47.84	kJ/mol	Joback Method
log10ws	-4.72		Crippen Method
logp	4.399		Crippen Method
mcvol	170.270	ml/mol	McGowan Method
pc	2537.93	kPa	Joback Method
rinpol	1366.00		NIST Webbook
rinpol	1366.00		NIST Webbook
tb	549.14	K	Joback Method
tc	793.41	K	Joback Method
tf	241.57	K	Joback Method
vc	0.608	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	398.51	J/mol×K	549.14	Joback Method
cpg	504.59	J/mol×K	752.70	Joback Method
cpg	486.40	J/mol×K	711.99	Joback Method
cpg	466.70	J/mol×K	671.27	Joback Method
cpg	445.48	J/mol×K	630.56	Joback Method
cpg	422.75	J/mol×K	589.85	Joback Method
cpg	521.25	J/mol×K	793.41	Joback Method
dvisc	0.0000478	Pa×s	549.14	Joback Method

dvisc	0.0000816	Pa×s	497.88	Joback Method
dvisc	0.0001573	Pa×s	446.62	Joback Method
dvisc	0.0003595	Pa×s	395.36	Joback Method
dvisc	0.0010515	Pa×s	344.09	Joback Method
dvisc	0.0044782	Pa×s	292.83	Joback Method
dvisc	0.0352747	Pa×s	241.57	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R3106&Units=SI
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

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