

cis,cis-2,11-tridecadiene

Inchi:	InChI=1S/C13H24/c1-3-5-7-9-11-13-12-10-8-6-4-2/h3-6H,7-13H2,1-2H3/b5-3-,6-4-
InchiKey:	YUSQM̱HV̱VYẔQX-GLIM̱PGKSA-N
Formula:	C13H24
SMILES:	CC=CCCCCCCCC=CC
Mol. weight [g/mol]:	180.33

Physical Properties

Property code	Value	Unit	Source
gf	219.02	kJ/mol	Joback Method
hf	-77.21	kJ/mol	Joback Method
hfus	29.83	kJ/mol	Joback Method
hvap	44.45	kJ/mol	Joback Method
log10ws	-4.97		Crippen Method
logp	4.869		Crippen Method
mcvol	185.430	ml/mol	McGowan Method
pc	1792.42	kPa	Joback Method
rinpol	1312.00		NIST Webbook
rinpol	1312.00		NIST Webbook
tb	505.16	K	Joback Method
tc	679.26	K	Joback Method
tf	226.11	K	Joback Method
vc	0.724	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	422.28	J/mol×K	505.16	Joback Method
cpg	499.96	J/mol×K	650.24	Joback Method
cpg	485.87	J/mol×K	621.23	Joback Method
cpg	471.09	J/mol×K	592.21	Joback Method
cpg	455.58	J/mol×K	563.19	Joback Method
cpg	439.33	J/mol×K	534.18	Joback Method
cpg	513.41	J/mol×K	679.26	Joback Method
dvisc	0.0001416	Pa×s	505.16	Joback Method

dvisc	0.0001908	Pa×s	458.65	Joback Method
dvisc	0.0002751	Pa×s	412.14	Joback Method
dvisc	0.0004354	Pa×s	365.63	Joback Method
dvisc	0.0007875	Pa×s	319.13	Joback Method
dvisc	0.0017438	Pa×s	272.62	Joback Method
dvisc	0.0053549	Pa×s	226.11	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R133874&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

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