

c-cyclotridecene

Inchi:	InChI=1S/C13H24/c1-2-4-6-8-10-12-13-11-9-7-5-3-1/h1-2H,3-13H2/b2-1-
InchiKey:	AVHHUCROZGSCGZ-UPHRSURJSA-N
Formula:	C13H24
SMILES:	C1=CCCCCCCCCCCC1
Mol. weight [g/mol]:	180.33

Physical Properties

Property code	Value	Unit	Source
gf	36.00	kJ/mol	Joback Method
hf	-222.33	kJ/mol	Joback Method
hfus	6.71	kJ/mol	Joback Method
hvap	46.77	kJ/mol	Joback Method
log10ws	-5.01		Crippen Method
logp	4.847		Crippen Method
mcvol	178.870	ml/mol	McGowan Method
pc	2458.04	kPa	Joback Method
rinpol	1401.30		NIST Webbook
tb	550.11	K	Joback Method
tc	797.26	K	Joback Method
tf	224.01	K	Joback Method
vc	0.627	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	437.00	J/mol×K	550.11	Joback Method
cpg	465.44	J/mol×K	591.30	Joback Method
cpg	492.10	J/mol×K	632.49	Joback Method
cpg	516.97	J/mol×K	673.69	Joback Method
cpg	540.04	J/mol×K	714.88	Joback Method
cpg	561.31	J/mol×K	756.07	Joback Method
cpg	580.75	J/mol×K	797.26	Joback Method
dvisc	0.2372933	Pa×s	224.01	Joback Method
dvisc	0.0133192	Pa×s	278.36	Joback Method

dvisc	0.0019157	Pa×s	332.71	Joback Method
dvisc	0.0004750	Pa×s	387.06	Joback Method
dvisc	0.0001660	Pa×s	441.41	Joback Method
dvisc	0.0000731	Pa×s	495.76	Joback Method
dvisc	0.0000378	Pa×s	550.11	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=R389225&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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