

Cycloundecene, 1-methyl-

Inchi:	InChI=1S/C12H22/c1-12-10-8-6-4-2-3-5-7-9-11-12/h10H,2-9,11H2,1H3/b12-10-
InchiKey:	IAGTWOIELUZWSL-BENRWUELSA-N
Formula:	C12H22
SMILES:	CC1=CCCCCCCCC1
Mol. weight [g/mol]:	166.30
CAS:	88828-82-4

Physical Properties

Property code	Value	Unit	Source
gf	42.15	kJ/mol	Joback Method
hf	-200.84	kJ/mol	Joback Method
hfus	7.93	kJ/mol	Joback Method
hvap	44.86	kJ/mol	Joback Method
log10ws	-4.59		Crippen Method
logp	4.457		Crippen Method
mcvol	164.780	ml/mol	McGowan Method
pc	2535.37	kPa	Joback Method
rinpol	1295.00		NIST Webbook
rinpol	1292.00		NIST Webbook
rinpol	1295.00		NIST Webbook
rinpol	1295.00		NIST Webbook
rinpol	1292.00		NIST Webbook
tb	523.67	K	Joback Method
tc	758.79	K	Joback Method
tf	232.30	K	Joback Method
vc	0.588	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	383.57	J/mol×K	523.67	Joback Method
cpg	408.47	J/mol×K	562.86	Joback Method
cpg	431.97	J/mol×K	602.04	Joback Method
cpg	454.07	J/mol×K	641.23	Joback Method

cpg	474.77	J/mol×K	680.41	Joback Method
cpg	494.08	J/mol×K	719.60	Joback Method
cpg	511.98	J/mol×K	758.79	Joback Method
dvisc	0.0489058	Pa×s	232.30	Joback Method
dvisc	0.0064003	Pa×s	280.86	Joback Method
dvisc	0.0015255	Pa×s	329.42	Joback Method
dvisc	0.0005256	Pa×s	377.99	Joback Method
dvisc	0.0002308	Pa×s	426.55	Joback Method
dvisc	0.0001199	Pa×s	475.11	Joback Method
dvisc	0.0000704	Pa×s	523.67	Joback Method

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307I
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=C88828824&Units=SI

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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