

CYCLOPENTANE, 2-n-OCTANYL-

Inchi:	InChI=1S/C13H24/c1-2-3-4-5-6-7-10-13-11-8-9-12-13/h8,11,13H,2-7,9-10,12H2,1H3
InchiKey:	SYEHHBWQHNEFBN-UHFFFAOYSA-N
Formula:	C13H24
SMILES:	CCCCCCCCC1C=CCC1
Mol. weight [g/mol]:	180.34

Physical Properties

Property code	Value	Unit	Source
af	0.4912		Cheméo Relay (1.0)
gf	125.09	kJ/mol	Joback Method
hf	-146.71	kJ/mol	Cheméo Relay (1.0)
hfus	24.58	kJ/mol	Joback Method
hvap	59.51	kJ/mol	Cheméo Relay (1.0)
ie	8.90	eV	Cheméo Relay (1.0)
log10ws	-6.14		Cheméo Relay (1.0)
logp	4.703		Crippen Method
mcvol	178.870	ml/mol	McGowan Method
pc	1975.31	kPa	Joback Method
rinpol	1309.00		NIST Webbook
tb	507.60	K	Cheméo Relay (1.0)
tc	684.10	K	Cheméo Relay (1.0)
tf	232.11	K	Cheméo Relay (1.0)
vc	0.680	m3/kmol	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	426.85	J/mol×K	511.28	Joback Method
cpg	446.28	J/mol×K	542.14	Joback Method
cpg	464.77	J/mol×K	572.99	Joback Method
cpg	482.35	J/mol×K	603.85	Joback Method
cpg	499.06	J/mol×K	634.71	Joback Method
cpg	514.93	J/mol×K	665.57	Joback Method
cpg	529.99	J/mol×K	696.42	Joback Method

dvisc	0.0044074	Pa×s	247.93	Joback Method
dvisc	0.0019436	Pa×s	291.82	Joback Method
dvisc	0.0010617	Pa×s	335.71	Joback Method
dvisc	0.0006670	Pa×s	379.61	Joback Method
dvisc	0.0004614	Pa×s	423.50	Joback Method
dvisc	0.0003421	Pa×s	467.39	Joback Method
dvisc	0.0002670	Pa×s	511.28	Joback Method

Sources

Joback Method:	https://en.wikipedia.org/wiki/Joback_method
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Cheméo Relay (1.0):	
Cheméo Relay (1.0, beta):	
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C66324489&Units=SI

Legend

af:	Acentric Factor
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
ie:	Ionization energy
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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