

Cyclooctane, 1,2-diethyl-

Other names:	1,2-Diethylcyclooctane
Inchi:	InChI=1S/C12H24/c1-3-11-9-7-5-6-8-10-12(11)4-2/h11-12H,3-10H2,1-2H3
InchiKey:	XDADRYBKGCGETX-UHFFFAOYSA-N
Formula:	C12H24
SMILES:	CCC1CCCCCCC1CC
Mol. weight [g/mol]:	168.32
CAS:	23609-46-3

Physical Properties

Property code	Value	Unit	Source
gf	42.70	kJ/mol	Joback Method
hf	-269.35	kJ/mol	Joback Method
hfus	15.54	kJ/mol	Joback Method
hvap	42.77	kJ/mol	Joback Method
log10ws	-4.26		Crippen Method
logp	4.393		Crippen Method
mcvol	169.080	ml/mol	McGowan Method
pc	2167.36	kPa	Joback Method
rinpol	1227.00		NIST Webbook
rinpol	1227.00		NIST Webbook
tb	497.38	K	Joback Method
tc	703.99	K	Joback Method
tf	221.10	K	Joback Method
vc	0.624	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	396.56	J/mol×K	497.38	Joback Method
cpg	503.20	J/mol×K	669.55	Joback Method
cpg	484.08	J/mol×K	635.12	Joback Method
cpg	463.87	J/mol×K	600.68	Joback Method
cpg	442.56	J/mol×K	566.25	Joback Method
cpg	420.12	J/mol×K	531.81	Joback Method

cpg	521.24	J/mol×K	703.99	Joback Method
dvisc	0.0001679	Pa×s	497.38	Joback Method
dvisc	0.0002400	Pa×s	451.33	Joback Method
dvisc	0.0003723	Pa×s	405.29	Joback Method
dvisc	0.0006463	Pa×s	359.24	Joback Method
dvisc	0.0013193	Pa×s	313.19	Joback Method
dvisc	0.0034442	Pa×s	267.15	Joback Method
dvisc	0.0134104	Pa×s	221.10	Joback Method

Sources

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=C23609463&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.cheméo.com/doc/models/crippen_log10ws

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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