

Cyclohexene, 3-(1-heptenyl)-4-(1,3-nonadienyl)-

Inchi:	InChI=1S/C22H36/c1-3-5-7-9-10-12-14-18-22-20-16-15-19-21(22)17-13-11-8-6-4-2/h10,1
InchiKey:	IQROVGHWWDUJID-HWMUKFTBSA-N
Formula:	C22H36
SMILES:	CCCCC=CC=CC1CCC=CC1C=CCCCC
Mol. weight [g/mol]:	300.52
CAS:	56318-85-5

Physical Properties

Property code	Value	Unit	Source
gf	421.72	kJ/mol	Joback Method
hf	-53.99	kJ/mol	Joback Method
hfus	47.47	kJ/mol	Joback Method
hvap	64.85	kJ/mol	Joback Method
log10ws	-7.86		Crippen Method
logp	7.398		Crippen Method
mcvol	292.780	ml/mol	McGowan Method
pc	1136.73	kPa	Joback Method
rinpol	2178.40		NIST Webbook
tb	729.28	K	Joback Method
tc	923.59	K	Joback Method
tf	326.36	K	Joback Method
vc	1.125	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	870.44	J/mol×K	729.28	Joback Method
cpg	892.51	J/mol×K	761.67	Joback Method
cpg	913.38	J/mol×K	794.05	Joback Method
cpg	933.13	J/mol×K	826.44	Joback Method
cpg	951.83	J/mol×K	858.82	Joback Method
cpg	969.55	J/mol×K	891.21	Joback Method
cpg	986.39	J/mol×K	923.59	Joback Method
dvisc	0.0023161	Pa×s	326.36	Joback Method

dvisc	0.0007759	Pa×s	393.51	Joback Method
dvisc	0.0003575	Pa×s	460.67	Joback Method
dvisc	0.0002007	Pa×s	527.82	Joback Method
dvisc	0.0001283	Pa×s	594.97	Joback Method
dvisc	0.0000898	Pa×s	662.13	Joback Method
dvisc	0.0000672	Pa×s	729.28	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=C56318855&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.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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