

Decane 3-cyclohexyl-, 3-cyclohexyl-

Other names:	(1-Ethyloctyl)cyclohexane Cyclohexane, 1-ethyloctyl
Inchi:	InChI=1S/C16H32/c1-3-5-6-7-9-12-15(4-2)16-13-10-8-11-14-16/h15-16H,3-14H2,1-2H3
InchiKey:	OUPADZQNAUCFAW-UHFFFAOYSA-N
Formula:	C16H32
SMILES:	CCCCCCCC(CC)C1CCCCC1
Mol. weight [g/mol]:	224.43

Physical Properties

Property code	Value	Unit	Source
af	0.5442		Cheméo Relay (1.0)
gf	105.85	kJ/mol	Joback Method
hf	-305.12	kJ/mol	Cheméo Relay (1.0)
hfus	25.51	kJ/mol	Joback Method
hvap	71.95	kJ/mol	Cheméo Relay (1.0)
ie	9.44	eV	Cheméo Relay (1.0)
logp	5.953		Crippen Method
mcvol	225.440	ml/mol	McGowan Method
pc	1548.78	kPa	Joback Method
rinpol	1625.00		NIST Webbook
rinpol	1625.00		NIST Webbook
tb	558.13	K	Cheméo Relay (1.0)
tc	743.51	K	Cheméo Relay (1.0)
tf	242.03	K	Cheméo Relay (1.0)
vc	0.820	m3/kmol	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	606.23	J/mol×K	584.59	Joback Method
cpg	629.24	J/mol×K	615.77	Joback Method
cpg	651.12	J/mol×K	646.95	Joback Method
cpg	671.90	J/mol×K	678.13	Joback Method
cpg	691.62	J/mol×K	709.31	Joback Method

cpg	710.30	J/mol×K	740.49	Joback Method
cpg	727.99	J/mol×K	771.67	Joback Method
dvisc	0.0097461	Pa×s	262.46	Joback Method
dvisc	0.0027083	Pa×s	316.15	Joback Method
dvisc	0.0010915	Pa×s	369.84	Joback Method
dvisc	0.0005539	Pa×s	423.52	Joback Method
dvisc	0.0003274	Pa×s	477.21	Joback Method
dvisc	0.0002153	Pa×s	530.90	Joback Method
dvisc	0.0001529	Pa×s	584.59	Joback Method

Sources

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=C13151741&Units=SI
Joback Method:	https://en.wikipedia.org/wiki/Joback_method

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
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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