

6-Chlorohex-1-ene

Other names:	6-Chloro-1-hexene
Inchi:	InChI=1S/C6H11Cl/c1-2-3-4-5-6-7/h2H,1,3-6H2
InchiKey:	BLMIXWDJHNJWDT-UHFFFAOYSA-N
Formula:	C6H11Cl
SMILES:	C=CCCCC(Cl)
Mol. weight [g/mol]:	118.61
CAS:	---

Physical Properties

Property code	Value	Unit	Source
af	0.3117		Cheméo Relay (1.0)
gf	75.55	kJ/mol	Joback Method
hf	-84.63	kJ/mol	Cheméo Relay (1.0)
hfus	14.21	kJ/mol	Joback Method
hvap	41.34	kJ/mol	Cheméo Relay (1.0)
ie	10.00	eV	Cheméo Relay (1.0)
log10ws	-2.87		Cheméo Relay (1.0)
logp	2.582		Crippen Method
mcvol	103.340	ml/mol	McGowan Method
pc	3124.49	kPa	Joback Method
rinpol	869.00		NIST Webbook
rinpol	869.00		NIST Webbook
tb	397.77	K	Cheméo Relay (1.0)
tc	587.42	K	Cheméo Relay (1.0)
tf	183.61	K	Cheméo Relay (1.0)
vc	0.371	m3/kmol	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	172.06	J/mol×K	370.79	Joback Method
cpg	224.57	J/mol×K	546.67	Joback Method
cpg	216.77	J/mol×K	517.35	Joback Method
cpg	208.61	J/mol×K	488.04	Joback Method

cpg	200.07	J/mol×K	458.73	Joback Method
cpg	191.14	J/mol×K	429.42	Joback Method
cpg	181.81	J/mol×K	400.10	Joback Method
dvisc	0.0006834	Pa×s	278.16	Joback Method
dvisc	0.0002830	Pa×s	370.79	Joback Method
dvisc	0.0003600	Pa×s	339.91	Joback Method
dvisc	0.0004803	Pa×s	309.04	Joback Method
dvisc	0.0039783	Pa×s	185.54	Joback Method
dvisc	0.0010617	Pa×s	247.29	Joback Method
dvisc	0.0018703	Pa×s	216.42	Joback Method

Correlations

Information	Value
Property code	pvap
Equation	$\ln(P_{vp}) = A + B/(T + C)$
Coeff. A	1.38357e+01
Coeff. B	-3.29167e+03
Coeff. C	-5.09180e+01
Temperature range (K), min.	293.88
Temperature range (K), max.	437.07

Sources

Cheméo Relay (1.0, beta):

The Yaws Handbook of Vapor
Pressure:
NIST Webbook:

<https://www.sciencedirect.com/book/9780128029992/the-yaws-handbook-of-vapor-pressure>

<http://webbook.nist.gov/cgi/cbook.cgi?ID=C928892&Units=SI>

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):

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
pvap:	Vapor 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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