

Heptane, 4-chloro-2-methyl

Inchi:	InChI=1S/C8H17Cl/c1-4-5-8(9)6-7(2)3/h7-8H,4-6H2,1-3H3
InchiKey:	NZPCEFUPEFPZSY-UHFFFAOYSA-N
Formula:	C8H17Cl
SMILES:	CCCC(Cl)CC(C)C
Mol. weight [g/mol]:	148.67

Physical Properties

Property code	Value	Unit	Source
gf	-0.33	kJ/mol	Joback Method
hf	-234.75	kJ/mol	Joback Method
hfus	13.63	kJ/mol	Joback Method
hvap	37.01	kJ/mol	Joback Method
log10ws	-3.19		Crippen Method
logp	3.440		Crippen Method
mcvol	135.820	ml/mol	McGowan Method
pc	2482.59	kPa	Joback Method
rinpol	953.00		NIST Webbook
rinpol	981.00		NIST Webbook
rinpol	953.00		NIST Webbook
rinpol	981.00		NIST Webbook
tb	418.99	K	Joback Method
tc	597.64	K	Joback Method
tf	179.84	K	Joback Method
vc	0.520	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	262.83	J/molxK	418.99	Joback Method
cpg	276.35	J/molxK	448.77	Joback Method
cpg	289.32	J/molxK	478.54	Joback Method
cpg	301.74	J/molxK	508.32	Joback Method
cpg	313.63	J/molxK	538.09	Joback Method
cpg	325.02	J/molxK	567.87	Joback Method

cpg	335.90	J/mol×K	597.64	Joback Method
dvisc	0.0164704	Paxs	179.84	Joback Method
dvisc	0.0043901	Paxs	219.70	Joback Method
dvisc	0.0017563	Paxs	259.56	Joback Method
dvisc	0.0008967	Paxs	299.42	Joback Method
dvisc	0.0005362	Paxs	339.27	Joback Method
dvisc	0.0003572	Paxs	379.13	Joback Method
dvisc	0.0002571	Paxs	418.99	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R116037&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

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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