

2-Chloro-2-methylheptane

Other names:	Heptane, 2-chloro-2-methyl-
Inchi:	InChI=1S/C8H17Cl/c1-4-5-6-7-8(2,3)9/h4-7H2,1-3H3
InchiKey:	VZYCLOQPZDXYHA-UHFFFAOYSA-N
Formula:	C8H17Cl
SMILES:	CCCCC(C)(C)Cl
Mol. weight [g/mol]:	148.67
CAS:	4325-49-9

Physical Properties

Property code	Value	Unit	Source
gf	7.39	kJ/mol	Joback Method
hf	-232.94	kJ/mol	Joback Method
hfus	13.26	kJ/mol	Joback Method
hvap	36.49	kJ/mol	Joback Method
log10ws	-3.44		Crippen Method
logp	3.584		Crippen Method
mcvol	135.820	ml/mol	McGowan Method
pc	2490.03	kPa	Joback Method
rinpol	949.00		NIST Webbook
rinpol	949.00		NIST Webbook
tb	416.64	K	Joback Method
tc	598.52	K	Joback Method
tf	212.26	K	Joback Method
vc	0.521	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	264.68	J/mol×K	416.64	Joback Method
cpg	278.85	J/mol×K	446.95	Joback Method
cpg	292.32	J/mol×K	477.27	Joback Method
cpg	305.11	J/mol×K	507.58	Joback Method
cpg	317.26	J/mol×K	537.89	Joback Method
cpg	328.78	J/mol×K	568.20	Joback Method

cpg	339.71	J/mol×K	598.52	Joback Method
dvisc	0.0090186	Paxs	212.26	Joback Method
dvisc	0.0034485	Paxs	246.32	Joback Method
dvisc	0.0016656	Paxs	280.39	Joback Method
dvisc	0.0009419	Paxs	314.45	Joback Method
dvisc	0.0005954	Paxs	348.51	Joback Method
dvisc	0.0004084	Paxs	382.58	Joback Method
dvisc	0.0002979	Paxs	416.64	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=C4325499&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307i
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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