Hexane, 2-chloro-2,5-dimethyl-

Other names: 2-Chloro-2,5-dimethylhexane
Inchi: InChI=1S/C8H17Cl/c1-7(2)5-6-8(3,4)9/h7H,5-6H2,1-4H3
InchiKey: SVRDRJZPEYTXKX-UHFFFAOYSA-N
Formula: C8H17Cl
SMILES: CC(C)CCC(C)(C)Cl
Mol. weight [g/mol]: 148.67
CAS: 29342-44-7

Physical Properties

Property code	Value	Unit	Source
gf	4.95	kJ/mol	Joback Method
hf	-238.22	kJ/mol	Joback Method
hfus	9.74	kJ/mol	Joback Method
hvap	36.10	kJ/mol	Joback Method
log10ws	-3.19		Crippen Method
logp	3.440		Crippen Method
mcvol	135.820	ml/mol	McGowan Method
pc	2510.03	kPa	Joback Method
tb	416.20	K	Joback Method
tc	602.32	K	Joback Method
tf	197.26	K	Joback Method
vc	0.515	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	264.66	J/mol×K	416.20	Joback Method
cpg	330.49	J/mol×K	571.30	Joback Method
cpg	318.69	J/mol×K	540.28	Joback Method
cpg	306.24	J/mol×K	509.26	Joback Method
cpg	293.11	J/mol×K	478.24	Joback Method
cpg	279.26	J/mol×K	447.22	Joback Method
cpg	341.66	J/mol×K	602.32	Joback Method
dvisc	0.0002864	Pa×s	416.20	Joback Method

dvisc	0.0004062	Pa×s	379.71	Joback Method
dvisc	0.0006206	Pa×s	343.22	Joback Method
dvisc	0.0010487	Pa×s	306.73	Joback Method
dvisc	0.0020416	Pa×s	270.24	Joback Method
dvisc	0.0048938	Pa×s	233.75	Joback Method
dvisc	0.0162102	Pa×s	197.26	Joback Method

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.43371e+01
Coeff. B	-3.77382e+03
Coeff. C	-6.35120e+01
Temperature range (K), min.	332.12
Temperature range (K), max.	481.63

Sources

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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C29342447&Units=SI
The Yaws Handbook of Vapor Pressure:	https://www.sciencedirect.com/book/9780128029992/the-yaws-handbook-of-vapor-pressure
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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
pvap:	Vapor pressure
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume