2-Chloro-2-methylpentane

Inchi: InChI=1S/C6H13Cl/c1-4-5-6(2,3)7/h4-5H2,1-3H3
InchiKey: NXXHAWKBICGUCK-UHFFFAOYSA-N
Formula: C6H13Cl
SMILES: CCCC(C)(C)Cl
Mol. weight [g/mol]: 120.62
CAS: 4325-48-8

Physical Properties

Property code	Value	Unit	Source
af	0.2715		Cheméo Relay (1.0)
gf	-9.45	kJ/mol	Joback Method
hf	-215.06	kJ/mol	Cheméo Relay (1.0)
hfl	-264.00 ± 2.00	kJ/mol	NIST Webbook
hfus	8.08	kJ/mol	Joback Method
hvap	36.22	kJ/mol	Cheméo Relay (1.0)
log10ws	-3.18		Cheméo Relay (1.0)
logp	2.804		Crippen Method
mcvol	107.640	ml/mol	McGowan Method
pc	3045.68	kPa	Joback Method
rinpol	807.00		NIST Webbook
rinpol	763.00		NIST Webbook
rinpol	807.00		NIST Webbook
rinpol	763.00		NIST Webbook
rinpol	766.54		NIST Webbook
rinpol	811.00		NIST Webbook
rinpol	767.00		NIST Webbook
rinpol	763.00		NIST Webbook
rinpol	766.54		NIST Webbook
ripol	899.00		NIST Webbook
ripol	916.00		NIST Webbook
ripol	898.00		NIST Webbook
tb	384.15 ± 3.00	K	NIST Webbook
tb	384.65 ± 2.00	K	NIST Webbook
tc	567.56	K	Cheméo Relay (1.0)
tf	192.38	K	Cheméo Relay (1.0)
vc	0.392	m3/kmol	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	187.00	J/mol×K	370.88	Joback Method
cpg	198.88	J/mol×K	401.54	Joback Method
cpg	210.15	J/mol×K	432.20	Joback Method
cpg	220.83	J/mol×K	462.87	Joback Method
cpg	230.95	J/mol×K	493.53	Joback Method
cpg	240.54	J/mol×K	524.19	Joback Method
cpg	249.61	J/mol×K	554.85	Joback Method
dvisc	0.0092209	Pa×s	189.72	Joback Method
dvisc	0.0036325	Pa×s	219.91	Joback Method
dvisc	0.0017919	Pa×s	250.11	Joback Method
dvisc	0.0010293	Pa×s	280.30	Joback Method
dvisc	0.0006585	Pa×s	310.49	Joback Method
dvisc	0.0004561	Pa×s	340.69	Joback Method
dvisc	0.0003353	Pa×s	370.88	Joback Method

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.55387e+01
Coeff. B	-3.67000e+03
Coeff. C	-4.80830e+01
Temperature range (K), min.	288.72
Temperature range (K), max.	406.93

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C4325488&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):	
Cheméo Relay (1.0, beta):	
The Yaws Handbook of Vapor Pressure:	https://www.sciencedirect.com/book/9780128029992/the-yaws-handbook-of-vapor-pressure

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
hfl:	Liquid phase 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
rinpol:	Non-polar retention indices
ripol:	Polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume