2-Chloro-2-methylnonane

Inchi: InChI=1S/C10H21Cl/c1-4-5-6-7-8-9-10(2,3)11/h4-9H2,1-3H3
InchiKey: QDJXQCKHBZEIJM-UHFFFAOYSA-N
Formula: C10H21Cl
SMILES: CCCCCCCC(C)(C)Cl
Mol. weight [g/mol]: 176.73
CAS: 4325-50-2

Physical Properties

Property code	Value	Unit	Source
gf	24.23	kJ/mol	Joback Method
hf	-274.22	kJ/mol	Joback Method
hfus	18.44	kJ/mol	Joback Method
hvap	40.94	kJ/mol	Joback Method
log10ws	-4.27		Crippen Method
logp	4.364		Crippen Method
mcvol	164.000	ml/mol	McGowan Method
pc	2073.65	kPa	Joback Method
tb	462.40	K	Joback Method
tc	641.37	K	Joback Method
tf	234.80	K	Joback Method
vc	0.633	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	350.93	J/mol×K	462.40	Joback Method
cpg	366.90	J/mol×K	492.23	Joback Method
cpg	382.10	J/mol×K	522.06	Joback Method
cpg	396.56	J/mol×K	551.89	Joback Method
cpg	410.30	J/mol×K	581.71	Joback Method
cpg	423.36	J/mol×K	611.54	Joback Method
cpg	435.78	J/mol×K	641.37	Joback Method
dvisc	0.0082387	Pa×s	234.80	Joback Method
dvisc	0.0030747	Pa×s	272.73	Joback Method

dvisc	0.0014598	Pa×s	310.67	Joback Method
dvisc	0.0008150	Pa×s	348.60	Joback Method
dvisc	0.0005102	Pa×s	386.53	Joback Method
dvisc	0.0003473	Pa×s	424.47	Joback Method
dvisc	0.0002518	Pa×s	462.40	Joback Method

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.38049e+01
Coeff. B	-3.90604e+03
Coeff. C	-7.43540e+01
Temperature range (K), min.	363.32
Temperature range (K), max.	534.24

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C4325502&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

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