1,1-Dichlorononane

Inchi: InChI=1S/C9H18Cl2/c1-2-3-4-5-6-7-8-9(10)11/h9H,2-8H2,1H3
InchiKey: FBTKIMWGAQACHU-UHFFFAOYSA-N
Formula: C9H18Cl2
SMILES: CCCCCCCCC(Cl)Cl
Mol. weight [g/mol]: 197.15
CAS: 821-88-5

Physical Properties

Property code	Value	Unit	Source
gf	-1.40	kJ/mol	Joback Method
hf	-265.85	kJ/mol	Joback Method
hfus	23.94	kJ/mol	Joback Method
hvap	44.01	kJ/mol	Joback Method
log10ws	-4.50		Crippen Method
logp	4.541		Crippen Method
mcvol	162.150	ml/mol	McGowan Method
pc	2167.36	kPa	Joback Method
rinpol	1291.00		NIST Webbook
tb	479.74	K	Joback Method
tc	659.36	K	Joback Method
tf	236.03	K	Joback Method
vc	0.631	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	335.36	J/mol×K	479.74	Joback Method
cpg	397.95	J/mol×K	629.42	Joback Method
cpg	386.57	J/mol×K	599.49	Joback Method
cpg	374.63	J/mol×K	569.55	Joback Method
cpg	362.13	J/mol×K	539.61	Joback Method
cpg	349.05	J/mol×K	509.68	Joback Method
cpg	408.80	J/mol×K	659.36	Joback Method
dvisc	0.0002575	Pa×s	479.74	Joback Method

dvisc	0.0003464	Pa×s	439.12	Joback Method
dvisc	0.0004951	Pa×s	398.50	Joback Method
dvisc	0.0007673	Pa×s	357.88	Joback Method
dvisc	0.0013304	Pa×s	317.27	Joback Method
dvisc	0.0027111	Pa×s	276.65	Joback Method
dvisc	0.0070588	Pa×s	236.03	Joback Method

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.47846e+01
Coeff. B	-4.42812e+03
Coeff. C	-8.04700e+01
Temperature range (K), min.	385.92
Temperature range (K), max.	547.91

Sources

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
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=R572531&Units=SI

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