1,2-Dichloro-3-methylbutane

Inchi: InChI=1S/C5H10Cl2/c1-4(2)5(7)3-6/h4-5H,3H2,1-2H3
InchiKey: FZGIQPIBNIFFDG-UHFFFAOYSA-N
Formula: C5H10Cl2
SMILES: CC(C)C(Cl)CCl
Mol. weight [g/mol]: 141.04
CAS: 600-10-2

Physical Properties

Property code	Value	Unit	Source
gf	-37.52	kJ/mol	Joback Method
hf	-188.57	kJ/mol	Joback Method
hfus	10.05	kJ/mol	Joback Method
hvap	34.72	kJ/mol	Joback Method
log10ws	-2.09		Crippen Method
logp	2.489		Crippen Method
mcvol	105.790	ml/mol	McGowan Method
pc	3243.03	kPa	Joback Method
rinpol	843.00		NIST Webbook
rinpol	838.00		NIST Webbook
tb	416.65 ± 2.00	K	NIST Webbook
tc	577.75	K	Joback Method
tf	175.95	K	Joback Method
vc	0.402	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	175.68	J/mol×K	387.78	Joback Method
cpg	185.11	J/mol×K	419.44	Joback Method
cpg	194.11	J/mol×K	451.10	Joback Method
cpg	202.69	J/mol×K	482.77	Joback Method
cpg	210.87	J/mol×K	514.43	Joback Method
cpg	218.66	J/mol×K	546.09	Joback Method
cpg	226.08	J/mol×K	577.75	Joback Method

dvisc	0.0132129	Pa×s	175.95	Joback Method
dvisc	0.0042286	Pa×s	211.25	Joback Method
dvisc	0.0018754	Pa×s	246.56	Joback Method
dvisc	0.0010197	Pa×s	281.87	Joback Method
dvisc	0.0006349	Pa×s	317.17	Joback Method
dvisc	0.0004347	Pa×s	352.48	Joback Method
dvisc	0.0003189	Pa×s	387.78	Joback Method

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.34158e+01
Coeff. B	-2.78522e+03
Coeff. C	-1.00055e+02
Temperature range (K), min.	312.21
Temperature range (K), max.	443.73

Sources

McGowan Method: http://link.springer.com/article/10.1007/BF02311772

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C600102&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

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