1,2-DICHLORO-2-METHYLPROPANE

Other names: 1,2-Dichloroisobutane
Isobutylene dichloride
Inchi: InChI=1S/C4H8Cl2/c1-4(2,6)3-5/h3H2,1-2H3
InchiKey: OQPNDCHKFIHPBY-UHFFFAOYSA-N
Formula: C4H8Cl2
SMILES: CC(C)(Cl)CCl
Mol. weight [g/mol]: 127.01
CAS: 594-37-6

Physical Properties

Property code	Value	Unit	Source
af	0.2482		Cheméo Relay (1.0)
gf	-38.22	kJ/mol	Joback Method
hf	-211.72	kJ/mol	Cheméo Relay (1.0)
hfus	7.10	kJ/mol	Joback Method
hvap	36.16	kJ/mol	Cheméo Relay (1.0)
ie	10.49	eV	Cheméo Relay (1.0)
log10ws	-2.45		Cheméo Relay (1.0)
logp	2.243		Crippen Method
mcvol	91.700	ml/mol	McGowan Method
pc	3642.13	kPa	Joback Method
rinpol	720.00		NIST Webbook
rinpol	720.00		NIST Webbook
rinpol	720.00		NIST Webbook
rinpol	733.00		NIST Webbook
rinpol	733.00		NIST Webbook
rinpol	733.00		NIST Webbook
rinpol	719.00		NIST Webbook
tb	379.00 ± 2.00	K	NIST Webbook
tb	379.15 ± 1.00	K	NIST Webbook
tb	380.15 ± 1.00	K	NIST Webbook
tb	378.65 ± 2.00	K	NIST Webbook
tb	380.15 ± 2.00	K	NIST Webbook
tb	381.00 ± 2.00	K	NIST Webbook
tb	380.15 ± 1.50	K	NIST Webbook
tb	379.70	K	NIST Webbook
tc	590.57	K	Cheméo Relay (1.0)

tf	230.81	K	Cheméo Relay (1.0)
vc	0.327	m3/kmol	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	142.86	J/mol×K	362.55	Joback Method
cpg	187.80	J/mol×K	557.27	Joback Method
cpg	181.49	J/mol×K	524.81	Joback Method
cpg	174.74	J/mol×K	492.36	Joback Method
cpg	167.53	J/mol×K	459.91	Joback Method
cpg	159.83	J/mol×K	427.46	Joback Method
cpg	151.62	J/mol×K	395.00	Joback Method
dvisc	0.0011406	Pa×s	279.83	Joback Method
dvisc	0.0004048	Pa×s	362.55	Joback Method
dvisc	0.0005402	Pa×s	334.98	Joback Method
dvisc	0.0007591	Pa×s	307.40	Joback Method
dvisc	0.0076660	Pa×s	197.10	Joback Method
dvisc	0.0018734	Pa×s	252.25	Joback Method
dvisc	0.0034758	Pa×s	224.68	Joback Method
hvapt	40.40	kJ/mol	314.00	NIST Webbook

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.32469e+01
Coeff. B	-2.47405e+03
Coeff. C	-9.32720e+01
Temperature range (K), min.	284.18
Temperature range (K), max.	405.05

Sources

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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C594376&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

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
hfus:	Enthalpy of fusion at standard conditions
hvap:	Enthalpy of vaporization at standard conditions
hvapt:	Enthalpy of vaporization at a given temperature
ie:	Ionization energy
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