

Butane, 1,3-dichloro-2-methyl-

Other names:	1,3-Dichloro-2-methylbutane
Inchi:	InChI=1S/C5H10Cl2/c1-4(3-6)5(2)7/h4-5H,3H2,1-2H3
InchiKey:	MCAJTVAYCDZHHF-UHFFFAOYSA-N
Formula:	C5H10Cl2
SMILES:	CC(Cl)C(C)CCl
Mol. weight [g/mol]:	141.04
CAS:	23010-07-3

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	874.00		NIST Webbook
rinpol	869.00		NIST Webbook
tb	387.78	K	Joback Method
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/molxK	387.78	Joback Method
cpg	185.11	J/molxK	419.44	Joback Method
cpg	194.11	J/molxK	451.10	Joback Method
cpg	202.69	J/molxK	482.77	Joback Method
cpg	210.87	J/molxK	514.43	Joback Method
cpg	218.66	J/molxK	546.09	Joback Method

cpg	226.08	J/mol×K	577.75	Joback Method
dvisc	0.0132129	Paxs	175.95	Joback Method
dvisc	0.0042286	Paxs	211.25	Joback Method
dvisc	0.0018754	Paxs	246.56	Joback Method
dvisc	0.0010197	Paxs	281.87	Joback Method
dvisc	0.0006349	Paxs	317.17	Joback Method
dvisc	0.0004347	Paxs	352.48	Joback Method
dvisc	0.0003189	Paxs	387.78	Joback Method

Correlations

Information	Value
Property code	pvap
Equation	$\ln(P_{vp}) = A + B/(T + C)$
Coeff. A	1.47169e+01
Coeff. B	-3.69507e+03
Coeff. C	-5.68400e+01
Temperature range (K), min.	312.92
Temperature range (K), max.	449.70

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C23010073&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/ci9903071
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
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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