

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

Other names:	2,3-Dichloro-2-methylbutane Amylene dichloride
Inchi:	InChI=1S/C5H10Cl2/c1-4(6)5(2,3)7/h4H,1-3H3
InchiKey:	TXTORVZCRUFBBO-UHFFFAOYSA-N
Formula:	C5H10Cl2
SMILES:	CC(Cl)C(C)(C)Cl
Mol. weight [g/mol]:	141.04
CAS:	507-45-9

Physical Properties

Property code	Value	Unit	Source
gf	-32.24	kJ/mol	Joback Method
hf	-192.04	kJ/mol	Joback Method
hfus	6.16	kJ/mol	Joback Method
hvap	33.81	kJ/mol	Joback Method
log10ws	-2.69		Aqueous Solubility Prediction Method
logp	2.631		Crippen Method
mcvol	105.790	ml/mol	McGowan Method
pc	3284.05	kPa	Joback Method
rinpola	844.00		NIST Webbook
rinpola	796.00		NIST Webbook
rinpola	790.00		NIST Webbook
tb	384.99	K	Joback Method
tc	583.40	K	Joback Method
tf	193.37	K	Joback Method
vc	0.397	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	177.35	J/molxK	384.99	Joback Method
cpg	187.87	J/molxK	418.06	Joback Method
cpg	197.76	J/molxK	451.13	Joback Method

cpg	207.03	J/mol×K	484.19	Joback Method
cpg	215.73	J/mol×K	517.26	Joback Method
cpg	223.89	J/mol×K	550.33	Joback Method
cpg	231.52	J/mol×K	583.40	Joback Method
dvisc	0.0136726	Paxs	193.37	Joback Method
dvisc	0.0048915	Paxs	225.31	Joback Method
dvisc	0.0022588	Paxs	257.24	Joback Method
dvisc	0.0012372	Paxs	289.18	Joback Method
dvisc	0.0007638	Paxs	321.12	Joback Method
dvisc	0.0005146	Paxs	353.05	Joback Method
dvisc	0.0003701	Paxs	384.99	Joback Method

Correlations

Information	Value
Property code	pvap
Equation	$\ln(P_{vp}) = A + B/(T + C)$
Coeff. A	1.06754e+01
Coeff. B	-1.68831e+03
Coeff. C	-1.44004e+02
Temperature range (K), min.	306.53
Temperature range (K), max.	458.76

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C507459&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
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
KDB:	https://www.thermo.com/research/kdb/hcprop/showprop.php?cmpid=1619
Aqueous Solubility Prediction Method:	http://onschallenge.wikispaces.com/file/view/AqueousDataset002.xlsx/351826032/AqueousDa
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
mccvol:	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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