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
rinpol	790.00		NIST Webbook
rinpol	796.00		NIST Webbook
rinpol	844.00		NIST Webbook
tb	384.99	K	Joback Method
tc	583.40	K	Joback Method
tf	193.37	K	Joback Method
vc	0.397	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	177.35	J/mol×K	384.99	Joback Method
cpg	187.87	J/mol×K	418.06	Joback Method
cpg	197.76	J/mol×K	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	Pa×s	193.37	Joback Method
dvisc	0.0048915	Pa×s	225.31	Joback Method
dvisc	0.0022588	Pa×s	257.24	Joback Method
dvisc	0.0012372	Pa×s	289.18	Joback Method
dvisc	0.0007638	Pa×s	321.12	Joback Method
dvisc	0.0005146	Pa×s	353.05	Joback Method
dvisc	0.0003701	Pa×s	384.99	Joback Method

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = 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/ci990307l
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
KDB:	https://www.cheric.org/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
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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