Butane, 2,3-dichloro-, (R*,S*)-

Other names: Butane, 2,3-dichloro-, meso-
meso-2,3-Dichlorobutane
Inchi: InChI=1S/C4H8Cl2/c1-3(5)4(2)6/h3-4H,1-2H3/t3-,4+
InchiKey: RMISVOPUIFJTEO-ZXZARUISSA-N
Formula: C4H8Cl2
SMILES: CC(Cl)C(C)Cl
Mol. weight [g/mol]: 127.01
CAS: 4028-56-2

Physical Properties

Property code	Value	Unit	Source
chl	-2523.90 ± 1.70	kJ/mol	NIST Webbook
gf	-45.94	kJ/mol	Joback Method
hf	-202.30 ± 1.70	kJ/mol	NIST Webbook
hfl	-240.80 ± 1.70	kJ/mol	NIST Webbook
hfus	7.46	kJ/mol	Joback Method
hvap	38.41 ± 0.07	kJ/mol	NIST Webbook
hvap	38.40	kJ/mol	NIST Webbook
log10ws	-2.03		Crippen Method
logp	2.241		Crippen Method
mcvol	91.700	ml/mol	McGowan Method
pc	3628.97	kPa	Joback Method
tb	364.90	K	Joback Method
tc	555.91	K	Joback Method
tf	164.68	K	Joback Method
vc	0.345	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	141.51	J/mol×K	364.90	Joback Method
cpg	149.43	J/mol×K	396.73	Joback Method
cpg	157.00	J/mol×K	428.57	Joback Method
cpg	164.21	J/mol×K	460.40	Joback Method

cpg	171.09	J/mol×K	492.24	Joback Method
cpg	177.64	J/mol×K	524.07	Joback Method
cpg	183.87	J/mol×K	555.91	Joback Method
dvisc	0.0130687	Pa×s	164.68	Joback Method
dvisc	0.0042176	Pa×s	198.05	Joback Method
dvisc	0.0018860	Pa×s	231.42	Joback Method
dvisc	0.0010331	Pa×s	264.79	Joback Method
dvisc	0.0006475	Pa×s	298.16	Joback Method
dvisc	0.0004458	Pa×s	331.53	Joback Method
dvisc	0.0003287	Pa×s	364.90	Joback Method

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.28363e+01
Coeff. B	-2.46981e+03
Coeff. C	-9.48930e+01
Temperature range (K), min.	291.71
Temperature range (K), max.	423.11

Sources

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

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C4028562&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

chl: Standard liquid enthalpy of combustion

cpg: Ideal gas heat capacity

dvisc: Dynamic viscosity

gf:	Standard Gibbs free energy of formation
hf:	Enthalpy of formation at standard conditions
hfl:	Liquid phase 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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume