

Butane, 2,3-dichloro-, (R*,R*)-(./-.)-

Other names:	(./-.)-2,3-Dichlorobutane Butane, 2,3-dichloro-, (./-.)- DL-2,3-Dichlorobutane racemic-2,3-Dichlorobutane threo-2,3-Dichlorobutane
Inchi:	InChI=1S/C4H8Cl2/c1-3(5)4(2)6/h3-4H,1-2H3/t3-,4-/m0/s1
InchiKey:	RMISVOPUIFJTEO-IMJSIDKUSA-N
Formula:	C4H8Cl2
SMILES:	CC(Cl)C(C)Cl
Mol. weight [g/mol]:	127.01
CAS:	2211-67-8

Physical Properties

Property code	Value	Unit	Source
chl	-2522.70 ± 1.70	kJ/mol	NIST Webbook
gf	-45.94	kJ/mol	Joback Method
hf	-202.20 ± 1.70	kJ/mol	NIST Webbook
hfl	-241.90 ± 1.70	kJ/mol	NIST Webbook
hfus	7.46	kJ/mol	Joback Method
hvap	39.73 ± 0.05	kJ/mol	NIST Webbook
hvap	39.70	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/molxK	364.90	Joback Method

cpg	149.43	J/molxK	396.73	Joback Method
cpg	157.00	J/molxK	428.57	Joback Method
cpg	164.21	J/molxK	460.40	Joback Method
cpg	171.09	J/molxK	492.24	Joback Method
cpg	177.64	J/molxK	524.07	Joback Method
cpg	183.87	J/molxK	555.91	Joback Method
dvisc	0.0130687	Paxs	164.68	Joback Method
dvisc	0.0042176	Paxs	198.05	Joback Method
dvisc	0.0018860	Paxs	231.42	Joback Method
dvisc	0.0010331	Paxs	264.79	Joback Method
dvisc	0.0006475	Paxs	298.16	Joback Method
dvisc	0.0004458	Paxs	331.53	Joback Method
dvisc	0.0003287	Paxs	364.90	Joback Method

Correlations

Information	Value
Property code	pvap
Equation	$\ln(P_{vp}) = A + B/(T + C)$
Coeff. A	1.31226e+01
Coeff. B	-2.54724e+03
Coeff. C	-9.59060e+01
Temperature range (K), min.	294.37
Temperature range (K), max.	422.01

Sources

Joback Method:	https://en.wikipedia.org/wiki/Joback_method
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C2211678&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

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

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