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-/m1/s1
InchiKey:	RMISVOPUIFJTEO-IMJSIDKUSA-N
Formula:	C4H8Cl2
SMILES:	C[C@@H](Cl)[C@@H](C)Cl
Mol. weight [g/mol]:	127.01
CAS:	2211-67-8

Physical Properties

Property code	Value	Unit	Source
af	0.2489		Cheméo Relay (1.0)
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	39.73 ± 0.05	kJ/mol	NIST Webbook
hvap	39.70	kJ/mol	NIST Webbook
hvap	39.70	kJ/mol	NIST Webbook
ie	10.83	eV	Cheméo Relay (1.0)
log10ws	-2.54		Cheméo Relay (1.0)
logp	2.241		Crippen Method
mcvol	91.700	ml/mol	McGowan Method
pc	3628.97	kPa	Joback Method
tb	393.55	K	Cheméo Relay (1.0)
tc	574.12	K	Cheméo Relay (1.0)
tf	233.92	K	Cheméo Relay (1.0)
vc	0.349	m3/kmol	Cheméo Relay (1.0)

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	1.31226e+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

Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws

Cheméo Relay (1.0):

Cheméo Relay (1.0, beta):

The Yaws Handbook of Vapor Pressure:	https://www.sciencedirect.com/book/9780128029992/the-yaws-handbook-of-vapor-pressure
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C2211678&Units=SI

Legend

af:	Acentric Factor
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
ie:	Ionization energy
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