

Butane, 1,4-diiodo-

Other names:	1,4-Diiodobutane 1,4-Diodobutane Tetramethylene diiodide Tetramethylene iodide
Inchi:	InChI=1S/C4H8I2/c5-3-1-2-4-6/h1-4H2
InchiKey:	ROUYUBHVBKMQO-UHFFFAOYSA-N
Formula:	C4H8I2
SMILES:	ICCCI
Mol. weight [g/mol]:	309.92
CAS:	628-21-7

Physical Properties

Property code	Value	Unit	Source
chl	-2687.40 ± 1.80	kJ/mol	NIST Webbook
gf	99.04	kJ/mol	Joback Method
hf	29.00 ± 2.10	kJ/mol	NIST Webbook
hfl	-30.00 ± 2.00	kJ/mol	NIST Webbook
hfus	14.93	kJ/mol	Joback Method
hvap	59.00 ± 0.60	kJ/mol	NIST Webbook
hvap	59.00	kJ/mol	NIST Webbook
log10ws	-3.39		Crippen Method
logp	2.637		Crippen Method
mcvol	118.860	ml/mol	McGowan Method
pc	3690.97	kPa	Joback Method
tb	477.20	K	Joback Method
tc	720.71	K	Joback Method
tf	279.10 ± 0.40	K	NIST Webbook
vc	0.435	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	174.43	J/mol×K	477.20	Joback Method
cpg	182.27	J/mol×K	517.79	Joback Method

cpg	189.54	J/mol×K	558.37	Joback Method
cpg	196.27	J/mol×K	598.96	Joback Method
cpg	202.52	J/mol×K	639.54	Joback Method
cpg	208.32	J/mol×K	680.13	Joback Method
cpg	213.73	J/mol×K	720.71	Joback Method
dvisc	0.0058612	Paxs	250.96	Joback Method
dvisc	0.0028313	Paxs	288.67	Joback Method
dvisc	0.0016181	Paxs	326.37	Joback Method
dvisc	0.0010384	Paxs	364.08	Joback Method
dvisc	0.0007242	Paxs	401.79	Joback Method
dvisc	0.0005373	Paxs	439.49	Joback Method
dvisc	0.0004179	Paxs	477.20	Joback Method

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	422.70	K	3.50	NIST Webbook

Correlations

Information	Value
Property code	pvap
Equation	$\ln(P_{vp}) = A + B/(T + C)$
Coeff. A	1.35236e+01
Coeff. B	-4.05400e+03
Coeff. C	-8.09140e+01
Temperature range (K), min.	387.20
Temperature range (K), max.	574.57

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=C628217&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.cheméo.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
tbrp:	Boiling point at reduced pressure
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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