

meso-2,3-dibromobutane

Other names:	Butane, 2,3-dibromo-, erythro Threo-2,3-dibromobutane erythro-2,3-Dibromobutane
Inchi:	InChI=1S/C4H8Br2/c1-3(5)4(2)6/h3-4H,1-2H3/t3-,4+
InchiKey:	BXXWFOGWXLJPPA-ZXZARUISSA-N
Formula:	C4H8Br2
SMILES:	CC(Br)C(C)Br
Mol. weight [g/mol]:	215.91
CAS:	5780-13-2

Physical Properties

Property code	Value	Unit	Source
gf	6.56	kJ/mol	Joback Method
hf	-101.60	kJ/mol	NIST Webbook
hfus	9.64	kJ/mol	Joback Method
hvap	46.44	kJ/mol	NIST Webbook
ie	10.16	eV	NIST Webbook
log10ws	-2.58		Crippen Method
logp	2.553		Crippen Method
mcvol	102.220	ml/mol	McGowan Method
pc	4769.39	kPa	Joback Method
rinpol	916.00		NIST Webbook
tb	430.50 ± 0.50	K	NIST Webbook
tb	430.50	K	NIST Webbook
tc	639.11	K	Joback Method
tf	224.44	K	Joback Method
vc	0.371	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	158.26	J/mol×K	422.36	Joback Method
cpg	166.58	J/mol×K	458.48	Joback Method
cpg	174.37	J/mol×K	494.61	Joback Method

cpg	181.67	J/mol×K	530.73	Joback Method
cpg	188.50	J/mol×K	566.86	Joback Method
cpg	194.90	J/mol×K	602.98	Joback Method
cpg	200.90	J/mol×K	639.11	Joback Method
dvisc	0.0065317	Paxs	224.44	Joback Method
dvisc	0.0030527	Paxs	257.43	Joback Method
dvisc	0.0016958	Paxs	290.41	Joback Method
dvisc	0.0010621	Paxs	323.40	Joback Method
dvisc	0.0007254	Paxs	356.39	Joback Method
dvisc	0.0005285	Paxs	389.37	Joback Method
dvisc	0.0004045	Paxs	422.36	Joback Method
hvapt	41.70	kJ/mol	352.50	NIST Webbook

Correlations

Information	Value
Property code	pvap
Equation	$\ln(P_{vp}) = A + B/(T + C)$
Coeff. A	1.41224e+01
Coeff. B	-3.08399e+03
Coeff. C	-1.06007e+02
Temperature range (K), min.	328.92
Temperature range (K), max.	456.03

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=C5780132&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

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
hvapt:	Enthalpy of vaporization at a given temperature
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
rinpola:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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