BUTANE, 1,2-DIBROMO-3-METHYL-

Other names: 1,2-Dibromo-3-methylbutane
Inchi: InChI=1S/C5H10Br2/c1-4(2)5(7)3-6/h4-5H,3H2,1-2H3
InchiKey: XCVOFNNXLRFMGX-UHFFFAOYSA-N
Formula: C5H10Br2
SMILES: CC(C)C(Br)CBr
Mol. weight [g/mol]: 229.94
CAS: 10288-13-8

Physical Properties

Property code	Value	Unit	Source
af	0.4445		Cheméo Relay (1.0)
hfus	12.23	kJ/mol	Joback Method
hvap	48.11	kJ/mol	Cheméo Relay (1.0)
ie	9.99	eV	Cheméo Relay (1.0)
log10ws	-3.22		Cheméo Relay (1.0)
logp	2.801		Crippen Method
mcvol	116.310	ml/mol	McGowan Method
pc	4194.74	kPa	Joback Method
tb	436.33	K	Cheméo Relay (1.0)
tc	649.59	K	Cheméo Relay (1.0)
tf	269.46	K	Cheméo Relay (1.0)
vc	0.401	m3/kmol	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	195.24	J/mol×K	445.24	Joback Method
cpg	204.99	J/mol×K	480.90	Joback Method
cpg	214.15	J/mol×K	516.56	Joback Method
cpg	222.76	J/mol×K	552.22	Joback Method
cpg	230.84	J/mol×K	587.88	Joback Method
cpg	238.42	J/mol×K	623.54	Joback Method
cpg	245.55	J/mol×K	659.19	Joback Method
dvisc	0.0063998	Pa×s	235.71	Joback Method

dvisc	0.0029311	Pa×s	270.63	Joback Method
dvisc	0.0016048	Pa×s	305.55	Joback Method
dvisc	0.0009942	Pa×s	340.48	Joback Method
dvisc	0.0006733	Pa×s	375.40	Joback Method
dvisc	0.0004872	Pa×s	410.32	Joback Method
dvisc	0.0003710	Pa×s	445.24	Joback Method

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.40155e+01
Coeff. B	-3.73043e+03
Coeff. C	-6.51800e+01
Temperature range (K), min.	336.92
Temperature range (K), max.	493.77

Sources

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=C10288138&Units=SI

Joback Method: https://en.wikipedia.org/wiki/Joback_method

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

Legend

af: Acentric Factor

cpg: Ideal gas heat capacity

dvisc: Dynamic viscosity

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