Butane, 1,3-dibromo-3-methyl-

Other names:	1,3-Dibromo-3-methylbutane
Inchi:	InChI=1S/C5H10Br2/c1-5(2,7)3-4-6/h3-4H2,1-2H3
InchiKey:	XMJFMQSXQQUJTQ-UHFFFAOYSA-N
Formula:	C5H10Br2
SMILES:	CC(C)(Br)CCBr
Mol. weight [g/mol]:	229.94
CAS:	24443-15-0

Physical Properties

Property code	Value	Unit	Source
gf	22.70	kJ/mol	Joback Method
hf	-102.62	kJ/mol	Joback Method
hfus	11.86	kJ/mol	Joback Method
hvap	38.30	kJ/mol	Joback Method
log10ws	-2.89		Crippen Method
logp	2.945		Crippen Method
mcvol	116.310	ml/mol	McGowan Method
pc	4211.09	kPa	Joback Method
tb	442.89	K	Joback Method
tc	661.07	K	Joback Method
tf	268.13	K	Joback Method
vc	0.428	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	197.85	J/mol×K	442.89	Joback Method
cpg	242.00	J/mol×K	624.70	Joback Method
cpg	234.49	J/mol×K	588.34	Joback Method
cpg	226.38	J/mol×K	551.98	Joback Method
cpg	217.61	J/mol×K	515.62	Joback Method
cpg	208.11	J/mol×K	479.25	Joback Method
cpg	248.94	J/mol×K	661.07	Joback Method
dvisc	0.0004197	Pa×s	442.89	Joback Method

dvisc	0.0005404	Pa×s	413.76	Joback Method
dvisc	0.0007231	Pa×s	384.64	Joback Method
dvisc	0.0010149	Pa×s	355.51	Joback Method
dvisc	0.0015133	Pa×s	326.38	Joback Method
dvisc	0.0024400	Pa×s	297.26	Joback Method
dvisc	0.0043647	Pa×s	268.13	Joback Method

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	347.70	K	2.10	NIST Webbook

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

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C24443150&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
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

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
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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