Benzene, 2-bromo-4-methyl-1-(1-methylethyl)-

Other names:	3-Bromo-4-isopropyltoluene
	Thymyl bromide
	p-Cymene, 3-bromo-
Inchi:	InChI=1S/C10H13Br/c1-7(2)9-5-4-8(3)6-10(9)11/h4-7H,1-3H3
InchiKey:	XMIWWDSQSRUTKQ-UHFFFAOYSA-N
Formula:	C10H13Br
SMILES:	Cc1ccc(C(C)C)c(Br)c1
Mol. weight [g/mol]:	213.11
CAS:	4478-10-8

Physical Properties

Property code	Value	Unit	Source
gf	138.35	kJ/mol	Joback Method
hf	-15.09	kJ/mol	Joback Method
hfus	16.68	kJ/mol	Joback Method
hvap	47.50	kJ/mol	Joback Method
log10ws	-4.30		Crippen Method
logp	3.881		Crippen Method
mcvol	145.500	ml/mol	McGowan Method
pc	3086.42	kPa	Joback Method
tb	507.25 ± 0.50	K	NIST Webbook
tc	758.86	K	Joback Method
tf	298.72	K	Joback Method
vc	0.543	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	298.50	J/mol×K	530.56	Joback Method
cpg	312.40	J/mol×K	568.61	Joback Method
cpg	325.46	J/mol×K	606.66	Joback Method
cpg	337.72	J/mol×K	644.71	Joback Method
cpg	349.20	J/mol×K	682.76	Joback Method
cpg	359.96	J/mol×K	720.81	Joback Method

cpg	370.02	J/mol×K	758.86	Joback Method
dvisc	0.0020742	Pa×s	298.72	Joback Method
dvisc	0.0011645	Pa×s	337.36	Joback Method
dvisc	0.0007362	Pa×s	376.00	Joback Method
dvisc	0.0005069	Pa×s	414.64	Joback Method
dvisc	0.0003720	Pa×s	453.28	Joback Method
dvisc	0.0002865	Pa×s	491.92	Joback Method
dvisc	0.0002293	Pa×s	530.56	Joback Method
hvapt	48.30	kJ/mol	455.00	NIST Webbook

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.60510e+01
Coeff. B	-5.79192e+03
Coeff. C	-6.09000e-01
Temperature range (K), min.	368.04
Temperature range (K), max.	539.92

Sources

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
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C4478108&Units=SI

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
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