4-Bromo-n-butylbenzene

Other names:	1-(4-bromophenyl)propane
	1-Brom-4-butylbenzen
	1-Bromo-4-butylbenzene
	Benzene, 1-bromo-4-butyl-
Inchi:	InChI=1S/C10H13Br/c1-2-3-4-9-5-7-10(11)8-6-9/h5-8H,2-4H2,1H3
InchiKey:	BRGVKVZXDWGJBX-UHFFFAOYSA-N
Formula:	C10H13Br
SMILES:	CCCCc1ccc(Br)cc1
Mol. weight [g/mol]:	213.11
CAS:	41492-05-1

Physical Properties

Property code	Value	Unit	Source
gf	150.42	kJ/mol	Joback Method
hf	1.66	kJ/mol	Joback Method
hfus	20.59	kJ/mol	Joback Method
hvap	47.23	kJ/mol	Joback Method
log10ws	-4.27		Crippen Method
logp	3.792		Crippen Method
mcvol	145.500	ml/mol	McGowan Method
pc	3110.57	kPa	Joback Method
tb	518.70 ± 0.30	K	NIST Webbook
tc	748.00	K	Joback Method
tf	247.50 ± 0.02	K	NIST Webbook
vc	0.549	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	298.37	J/mol×K	526.02	Joback Method
cpg	359.58	J/mol×K	711.00	Joback Method
cpg	348.89	J/mol×K	674.01	Joback Method
cpg	337.46	J/mol×K	637.01	Joback Method
cpg	325.27	J/mol×K	600.01	Joback Method

cpg	312.25	J/mol×K	563.02	Joback Method
cpg	369.58	J/mol×K	748.00	Joback Method
dvisc	0.0002509	Pa×s	526.02	Joback Method
dvisc	0.0003131	Pa×s	488.55	Joback Method
dvisc	0.0004054	Pa×s	451.08	Joback Method
dvisc	0.0005500	Pa×s	413.61	Joback Method
dvisc	0.0007929	Pa×s	376.14	Joback Method
dvisc	0.0012395	Pa×s	338.67	Joback Method
dvisc	0.0021656	Pa×s	301.20	Joback Method

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.40884e+01
Coeff. B	-4.10846e+03
Coeff. C	-8.48620e+01
Temperature range (K), min.	382.56
Temperature range (K), max.	552.96

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=C41492051&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
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