1-Bromo-4-butylbenzene

Other names: 1-(4-bromophenyl)propane
1-Brom-4-butylbenzen
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]: 213.12
CAS: 41492-05-1

Physical Properties

Property code	Value	Unit	Source
af	0.4365		Cheméo Relay (1.0)
gf	150.42	kJ/mol	Joback Method
hf	9.74	kJ/mol	Cheméo Relay (1.0)
hfus	20.59	kJ/mol	Joback Method
hvap	60.33	kJ/mol	Cheméo Relay (1.0)
ie	8.71	eV	Cheméo Relay (1.0)
log10ws	-4.97		Cheméo Relay (1.0)
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	715.08	K	Cheméo Relay (1.0)
tf	247.50 ± 0.02	K	NIST Webbook
vc	0.535	m3/kmol	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	298.37	J/mol×K	526.02	Joback Method
cpg	312.25	J/mol×K	563.02	Joback Method
cpg	325.27	J/mol×K	600.01	Joback Method
cpg	337.46	J/mol×K	637.01	Joback Method

cpg	348.89	J/mol×K	674.01	Joback Method
cpg	359.58	J/mol×K	711.00	Joback Method
cpg	369.58	J/mol×K	748.00	Joback Method
dvisc	0.0021656	Pa×s	301.20	Joback Method
dvisc	0.0012395	Pa×s	338.67	Joback Method
dvisc	0.0007929	Pa×s	376.14	Joback Method
dvisc	0.0005500	Pa×s	413.61	Joback Method
dvisc	0.0004054	Pa×s	451.08	Joback Method
dvisc	0.0003131	Pa×s	488.55	Joback Method
dvisc	0.0002509	Pa×s	526.02	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

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=C41492051&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
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
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