p-tert-Butylbenzyl bromide

Other names:	1-(bromomethyl)-4-(1,1-dimethylethyl)benzene
	4-tert-Butylbenzyl bromide
	Benzene, 1-(bromomethyl)-4-(1,1-dimethylethyl)-
Inchi:	InChI=1S/C11H15Br/c1-11(2,3)10-6-4-9(8-12)5-7-10/h4-7H,8H2,1-3H3
InchiKey:	QZNQSIHCDAGZIA-UHFFFAOYSA-N
Formula:	C11H15Br
SMILES:	CC(C)(C)c1ccc(CBr)cc1
Mol. weight [g/mol]:	227.14
CAS:	18880-00-7

Physical Properties

Property code	Value	Unit	Source
gf	161.68	kJ/mol	Joback Method
hf	-27.73	kJ/mol	Joback Method
hfus	15.77	kJ/mol	Joback Method
hvap	48.16	kJ/mol	Joback Method
log10ws	-4.10		Crippen Method
logp	3.879		Crippen Method
mcvol	159.590	ml/mol	McGowan Method
pc	2859.68	kPa	Joback Method
tb	545.67	K	Joback Method
tc	778.11	K	Joback Method
tf	314.89	K	Joback Method
vc	0.595	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	347.24	J/mol×K	545.67	Joback Method
cpg	363.03	J/mol×K	584.41	Joback Method
cpg	377.66	J/mol×K	623.15	Joback Method
cpg	391.22	J/mol×K	661.89	Joback Method
cpg	403.78	J/mol×K	700.63	Joback Method
cpg	415.42	J/mol×K	739.37	Joback Method

cpg	426.22	J/mol×K	778.11	Joback Method
dvisc	0.0025782	Pa×s	314.89	Joback Method
dvisc	0.0013584	Pa×s	353.35	Joback Method
dvisc	0.0008117	Pa×s	391.82	Joback Method
dvisc	0.0005318	Pa×s	430.28	Joback Method
dvisc	0.0003734	Pa×s	468.74	Joback Method
dvisc	0.0002767	Pa×s	507.21	Joback Method
dvisc	0.0002138	Pa×s	545.67	Joback Method

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	366.70	K	0.10	NIST Webbook

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.16792e+01
Coeff. B	-3.46290e+03
Coeff. C	-8.82120e+01
Temperature range (K), min.	392.20
Temperature range (K), max.	632.04

Sources

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=C18880007&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

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