

3-tert-butylbromobenzene

Other names:	m-bromo-tert-butylbenzene
Inchi:	InChI=1S/C10H13Br/c1-10(2,3)8-5-4-6-9(11)7-8/h4-7H,1-3H3
InchiKey:	FDXXHPYFJDKWJS-UHFFFAOYSA-N
Formula:	C10H13Br
SMILES:	CC(C)(C)c1cccc(Br)c1
Mol. weight [g/mol]:	213.11
CAS:	3972-64-3

Physical Properties

Property code	Value	Unit	Source
gf	153.26	kJ/mol	Joback Method
hf	-7.09	kJ/mol	Joback Method
hfus	13.18	kJ/mol	Joback Method
hvap	45.93	kJ/mol	Joback Method
log10ws	-3.95		Crippen Method
logp	3.747		Crippen Method
mcvol	145.500	ml/mol	McGowan Method
pc	3177.55	kPa	Joback Method
tb	522.79	K	Joback Method
tc	759.79	K	Joback Method
tf	303.62	K	Joback Method
vc	0.538	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	301.75	J/mol×K	522.79	Joback Method
cpg	316.73	J/mol×K	562.29	Joback Method
cpg	330.58	J/mol×K	601.79	Joback Method
cpg	343.36	J/mol×K	641.29	Joback Method
cpg	355.16	J/mol×K	680.79	Joback Method
cpg	366.06	J/mol×K	720.29	Joback Method
cpg	376.13	J/mol×K	759.79	Joback Method
dvisc	0.0026932	Paxs	303.62	Joback Method

dvisc	0.0014454	Paxs	340.15	Joback Method
dvisc	0.0008753	Paxs	376.68	Joback Method
dvisc	0.0005792	Paxs	413.20	Joback Method
dvisc	0.0004098	Paxs	449.73	Joback Method
dvisc	0.0003055	Paxs	486.26	Joback Method
dvisc	0.0002372	Paxs	522.79	Joback Method

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
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=C3972643&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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

Latest version available from:

<https://www.chemeo.com/cid/75-575-1/3-tert-butylbromobenzene.pdf>

Generated by Cheméo on 2024-04-20 14:43:11.70758205 +0000 UTC m=+15913440.628159366.

Cheméo (<https://www.chemeo.com>) is the biggest free database of chemical and physical data for the process industry.