

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]:	213.12

Physical Properties

Property code	Value	Unit	Source
af	0.3338		Cheméo Relay (1.0)
hf	-7.52	kJ/mol	Cheméo Relay (1.0)
hfus	13.18	kJ/mol	Joback Method
hvap	56.73	kJ/mol	Cheméo Relay (1.0)
ie	8.79	eV	Cheméo Relay (1.0)
log10ws	-5.01		Cheméo Relay (1.0)
logp	3.747		Crippen Method
mcvol	145.500	ml/mol	McGowan Method
pc	3177.55	kPa	Joback Method
tb	498.71	K	Cheméo Relay (1.0)
tc	715.65	K	Cheméo Relay (1.0)
tf	262.28	K	Cheméo Relay (1.0)

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	Pa×s	303.62	Joback Method
dvisc	0.0014454	Pa×s	340.15	Joback Method

dvisc	0.0008753	Pa×s	376.68	Joback Method
dvisc	0.0005792	Pa×s	413.20	Joback Method
dvisc	0.0004098	Pa×s	449.73	Joback Method
dvisc	0.0003055	Pa×s	486.26	Joback Method
dvisc	0.0002372	Pa×s	522.79	Joback Method

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):	
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C3972643&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
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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point

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