5-t-Butyl-1,2,3-trimethylbenzene

Other names:	5-tert-Butyl-1,2,3-trimethylbenzene
	1-tert-Butyl-3,4,5-trimethyl-benzene
	Benzene, 5-(1,1-dimethylethyl)-1,2,3-trimethyl-
Inchi:	InChI=1S/C13H20/c1-9-7-12(13(4,5)6)8-10(2)11(9)3/h7-8H,1-6H3
InchiKey:	ZQVJKYPEIPJEIP-UHFFFAOYSA-N
Formula:	C13H20
SMILES:	Cc1cc(C(C)(C)C)cc(C)c1C
Mol. weight [g/mol]:	176.30
CAS:	98-23-7

Physical Properties

Property code	Value	Unit	Source
gf	144.94	kJ/mol	Joback Method
hf	-118.28	kJ/mol	Joback Method
hfus	14.89	kJ/mol	Joback Method
hvap	47.50	kJ/mol	Joback Method
log10ws	-4.21		Crippen Method
logp	3.909		Crippen Method
mcvol	170.270	ml/mol	McGowan Method
pc	2141.36	kPa	Joback Method
rinpol	1307.00		NIST Webbook
rinpol	1307.00		NIST Webbook
rinpol	1307.00		NIST Webbook
tb	535.23	K	Joback Method
tc	747.59	K	Joback Method
tf	302.67	K	Joback Method
vc	0.644	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	397.43	J/mol×K	535.23	Joback Method
cpg	415.20	J/mol×K	570.62	Joback Method
cpg	431.96	J/mol×K	606.02	Joback Method

cpg	447.77	J/mol×K	641.41	Joback Method
cpg	462.65	J/mol×K	676.81	Joback Method
cpg	476.67	J/mol×K	712.20	Joback Method
cpg	489.86	J/mol×K	747.59	Joback Method
dvisc	0.0017896	Pa×s	302.67	Joback Method
dvisc	0.0009621	Pa×s	341.43	Joback Method
dvisc	0.0005870	Pa×s	380.19	Joback Method
dvisc	0.0003924	Pa×s	418.95	Joback Method
dvisc	0.0002809	Pa×s	457.71	Joback Method
dvisc	0.0002118	Pa×s	496.47	Joback Method
dvisc	0.0001664	Pa×s	535.23	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C98237&Units=SI
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

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
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume