Benzene, 1-(1,1-dimethylethyl)-3-ethyl-5-methyl-

Other names: 1-tert-Butyl-3-ethyl-5-methylbenzene
3-tert-Butyl-5-ethyltoluene
Inchi: InChI=1S/C13H20/c1-6-11-7-10(2)8-12(9-11)13(3,4)5/h7-9H,6H2,1-5H3
InchiKey: URDKTSKLGNWKDB-UHFFFAOYSA-N
Formula: C13H20
SMILES: CCc1cc(C)cc(C(C)(C)C)c1
Mol. weight [g/mol]: 176.30
CAS: 6630-01-9

Physical Properties

Property code	Value	Unit	Source
gf	154.57	kJ/mol	Joback Method
hf	-106.81	kJ/mol	Joback Method
hfus	15.28	kJ/mol	Joback Method
hvap	46.84	kJ/mol	Joback Method
log10ws	-4.06		Crippen Method
logp	3.855		Crippen Method
mcvol	170.270	ml/mol	McGowan Method
pc	2171.40	kPa	Joback Method
rinpol	1238.30		NIST Webbook
rinpol	1238.30		NIST Webbook
tb	494.10 ± 0.40	K	NIST Webbook
tc	741.50	K	Joback Method
tf	290.15	K	Joback Method
vc	0.644	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	396.95	J/mol×K	530.25	Joback Method
cpg	477.43	J/mol×K	706.29	Joback Method
cpg	463.26	J/mol×K	671.08	Joback Method
cpg	448.17	J/mol×K	635.87	Joback Method
cpg	432.13	J/mol×K	600.67	Joback Method

cpg	415.07	J/mol×K	565.46	Joback Method
cpg	490.74	J/mol×K	741.50	Joback Method
dvisc	0.0001717	Pa×s	530.25	Joback Method
dvisc	0.0002233	Pa×s	490.23	Joback Method
dvisc	0.0003043	Pa×s	450.22	Joback Method
dvisc	0.0004403	Pa×s	410.20	Joback Method
dvisc	0.0006903	Pa×s	370.18	Joback Method
dvisc	0.0012067	Pa×s	330.17	Joback Method
dvisc	0.0024609	Pa×s	290.15	Joback Method

Sources

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
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C6630019&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
rinpol: Non-polar retention indices
tb: Normal Boiling Point Temperature
tc: Critical Temperature
tf: Normal melting (fusion) point
vc: Critical Volume