Benzene, 1-chloro-3,5-bis(1,1-dimethylethyl)-

Other names: 3,5-Di-tert-butyl chlorobenzene
Inchi: InChI=1S/C14H21Cl/c1-13(2,3)10-7-11(14(4,5)6)9-12(15)8-10/h7-9H,1-6H3
InchiKey: UMPNQCBQSXTKID-UHFFFAOYSA-N
Formula: C14H21Cl
SMILES: CC(C)(C)c1cc(Cl)cc(C(C)(C)C)c1
Mol. weight [g/mol]: 224.77
CAS: 80438-67-1

Physical Properties

Property code	Value	Unit	Source
gf	153.90	kJ/mol	Joback Method
hf	-151.94	kJ/mol	Joback Method
hfl	-229.00 ± 2.00	kJ/mol	NIST Webbook
hfus	14.65	kJ/mol	Joback Method
hvap	52.15	kJ/mol	Joback Method
log10ws	-4.78		Crippen Method
logp	4.935		Crippen Method
mcvol	196.600	ml/mol	McGowan Method
pc	1957.87	kPa	Joback Method
tb	587.33	K	Joback Method
tc	812.50	K	Joback Method
tf	333.76	K	Joback Method
vc	0.739	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	480.72	J/mol×K	587.33	Joback Method
cpg	561.64	J/mol×K	774.98	Joback Method
cpg	547.73	J/mol×K	737.45	Joback Method
cpg	532.77	J/mol×K	699.92	Joback Method
cpg	516.67	J/mol×K	662.39	Joback Method
cpg	499.35	J/mol×K	624.86	Joback Method
cpg	574.60	J/mol×K	812.50	Joback Method

dvisc	0.0001357	Pa×s	587.33	Joback Method
dvisc	0.0001818	Pa×s	545.07	Joback Method
dvisc	0.0002557	Pa×s	502.81	Joback Method
dvisc	0.0003828	Pa×s	460.54	Joback Method
dvisc	0.0006219	Pa×s	418.28	Joback Method
dvisc	0.0011269	Pa×s	376.02	Joback Method
dvisc	0.0023734	Pa×s	333.76	Joback Method

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.11942e+01
Coeff. B	-3.33206e+03
Coeff. C	-8.84900e+01
Temperature range (K), min.	394.00
Temperature range (K), max.	654.91

Sources

McGowan Method: http://link.springer.com/article/10.1007/BF02311772

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C80438671&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

Joback Method: https://en.wikipedia.org/wiki/Joback_method

Legend

cpg: Ideal gas heat capacity

dvisc: Dynamic viscosity

gf: Standard Gibbs free energy of formation

hf: Enthalpy of formation at standard conditions

hfl: Liquid phase 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
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume