

Benzene, 1,3,5-trichloro-2,4,6-trimethyl-

Other names:	Mesitylene, 2,4,6-trichloro- 2,4,6-Trichloromesitylene 1,3,5-Trichloro-2,4,6-trimethylbenzene
Inchi:	InChI=1S/C9H9Cl3/c1-4-7(10)5(2)9(12)6(3)8(4)11/h1-3H3
InchiKey:	VMNISWKTOHUZQN-UHFFFAOYSA-N
Formula:	C9H9Cl3
SMILES:	Cc1c(Cl)c(C)c(Cl)c(C)c1Cl
Mol. weight [g/mol]:	223.53
CAS:	5324-68-5

Physical Properties

Property code	Value	Unit	Source
gf	53.37	kJ/mol	Joback Method
hf	-97.13	kJ/mol	Joback Method
hfus	23.75	kJ/mol	Joback Method
hvap	54.37	kJ/mol	Joback Method
log10ws	-4.95		Crippen Method
logp	4.572		Crippen Method
mcvol	150.630	ml/mol	McGowan Method
pc	2665.27	kPa	Joback Method
tb	569.19	K	Joback Method
tc	798.82	K	Joback Method
tf	369.97	K	Joback Method
vc	0.579	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	289.35	J/molxK	569.19	Joback Method
cpg	299.51	J/molxK	607.46	Joback Method
cpg	309.13	J/molxK	645.73	Joback Method
cpg	318.24	J/molxK	684.00	Joback Method
cpg	326.84	J/molxK	722.27	Joback Method
cpg	334.94	J/molxK	760.55	Joback Method

cpg	342.55	J/mol×K	798.82	Joback Method
cps	232.39	J/mol×K	300.00	NIST Webbook
dvisc	0.0009091	Paxs	369.97	Joback Method
dvisc	0.0006585	Paxs	403.17	Joback Method
dvisc	0.0005009	Paxs	436.38	Joback Method
dvisc	0.0003961	Paxs	469.58	Joback Method
dvisc	0.0003231	Paxs	502.78	Joback Method
dvisc	0.0002703	Paxs	535.99	Joback Method
dvisc	0.0002308	Paxs	569.19	Joback Method

Sources

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=C5324685&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071

Legend

cpg:	Ideal gas heat capacity
cps:	Solid phase 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

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