

Benzene, 2-chloro-1,3-dimethyl-

Other names:	1-Chloro-2,6-dimethylbenzene 2,6-Dimethylchlorobenzene 2,6-Dimethylphenyl chloride 2-Chloro-1,3-dimethylbenzene 2-Chloro-m-xylene m-Xylene, 2-chloro-
Inchi:	InChI=1S/C8H9Cl/c1-6-4-3-5-7(2)8(6)9/h3-5H,1-2H3
InchiKey:	VDXLAYAQGYCQEO-UHFFFAOYSA-N
Formula:	C8H9Cl
SMILES:	Cc1cccc(C)c1Cl
Mol. weight [g/mol]:	140.61
CAS:	6781-98-2

Physical Properties

Property code	Value	Unit	Source
gf	97.70	kJ/mol	Joback Method
hf	-10.60	kJ/mol	Joback Method
hfus	13.94	kJ/mol	Joback Method
hvap	41.39	kJ/mol	Joback Method
log10ws	-3.11		Crippen Method
logp	2.957		Crippen Method
mcvol	112.060	ml/mol	McGowan Method
pc	3372.36	kPa	Joback Method
rinpol	1050.00		NIST Webbook
rinpol	1056.00		NIST Webbook
tb	455.70	K	NIST Webbook
tb	459.20	K	NIST Webbook
tc	676.11	K	Joback Method
tf	261.30	K	Joback Method
vc	0.424	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
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cpg	261.31	J/molxK	676.11	Joback Method
cpg	213.88	J/molxK	493.11	Joback Method
cpg	224.50	J/molxK	529.71	Joback Method
cpg	234.54	J/molxK	566.31	Joback Method
cpg	244.00	J/molxK	602.91	Joback Method
cpg	252.92	J/molxK	639.51	Joback Method
cpg	202.65	J/molxK	456.51	Joback Method
dvisc	0.0002952	Paxs	423.98	Joback Method
dvisc	0.0003710	Paxs	391.44	Joback Method
dvisc	0.0004860	Paxs	358.90	Joback Method
dvisc	0.0006718	Paxs	326.37	Joback Method
dvisc	0.0009978	Paxs	293.84	Joback Method
dvisc	0.0002426	Paxs	456.51	Joback Method
dvisc	0.0016353	Paxs	261.30	Joback Method
pvap	0.06	kPa	287.20	Vaporization enthalpies of a series of the fluoro- and chloro-substituted methylbenzenes
pvap	0.09	kPa	293.30	Vaporization enthalpies of a series of the fluoro- and chloro-substituted methylbenzenes
pvap	0.11	kPa	296.30	Vaporization enthalpies of a series of the fluoro- and chloro-substituted methylbenzenes
pvap	0.13	kPa	298.20	Vaporization enthalpies of a series of the fluoro- and chloro-substituted methylbenzenes
pvap	0.13	kPa	298.30	Vaporization enthalpies of a series of the fluoro- and chloro-substituted methylbenzenes
pvap	0.13	kPa	298.30	Vaporization enthalpies of a series of the fluoro- and chloro-substituted methylbenzenes
pvap	0.15	kPa	300.40	Vaporization enthalpies of a series of the fluoro- and chloro-substituted methylbenzenes

pvap	0.21	kPa	305.40	Vaporization enthalpies of a series of the fluoro- and chloro-substituted methylbenzenes
pvap	0.06	kPa	287.10	Vaporization enthalpies of a series of the fluoro- and chloro-substituted methylbenzenes
pvap	0.05	kPa	284.10	Vaporization enthalpies of a series of the fluoro- and chloro-substituted methylbenzenes
pvap	0.04	kPa	282.20	Vaporization enthalpies of a series of the fluoro- and chloro-substituted methylbenzenes
pvap	0.03	kPa	279.20	Vaporization enthalpies of a series of the fluoro- and chloro-substituted methylbenzenes
pvap	0.03	kPa	276.20	Vaporization enthalpies of a series of the fluoro- and chloro-substituted methylbenzenes
pvap	0.02	kPa	274.50	Vaporization enthalpies of a series of the fluoro- and chloro-substituted methylbenzenes
pvap	0.07	kPa	290.10	Vaporization enthalpies of a series of the fluoro- and chloro-substituted methylbenzenes

Correlations

Information	Value
Property code	pvap
Equation	$\ln(P_{vp}) = A + B/(T + C)$
Coeff. A	1.44419e+01

Coeff. B	-3.80081e+03
Coeff. C	-6.87940e+01
Temperature range (K), min.	337.32
Temperature range (K), max.	485.07

Sources

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=C6781982&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/ci990307I
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Vaporization enthalpies of a series of the fluoro- and chloro-substituted methylbenzenes:	https://www.doi.org/10.1016/j.fluid.2014.07.029

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

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