

Benzene, 1-(dichloromethyl)-4-methyl-

Other names:	1-(Dichloromethyl)-4-methylbenzene 4-Methyl-1-(dichloromethyl)benzene p-Methylbenzal chloride p-Xylene, «alpha», «alpha»-dichloro- p-Xylene, Â«alphaÂ», Â«alphaÂ»-dichloro-
Inchi:	InChI=1S/C8H8Cl2/c1-6-2-4-7(5-3-6)8(9)10/h2-5,8H,1H3
InchiKey:	RGDYIHSZBVIIND-UHFFFAOYSA-N
Formula:	C8H8Cl2
SMILES:	Cc1ccc(C(Cl)Cl)cc1
Mol. weight [g/mol]:	175.06
CAS:	23063-36-7

Physical Properties

Property code	Value	Unit	Source
gf	92.96	kJ/mol	Joback Method
hf	-20.15	kJ/mol	Joback Method
hfus	15.00	kJ/mol	Joback Method
hvap	44.72	kJ/mol	Joback Method
log10ws	-3.59		Crippen Method
logp	3.471		Crippen Method
mcvol	124.300	ml/mol	McGowan Method
pc	3318.18	kPa	Joback Method
tb	488.52	K	Joback Method
tc	718.20	K	Joback Method
tf	263.70	K	Joback Method
vc	0.468	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	226.94	J/molxK	488.52	Joback Method
cpg	238.34	J/molxK	526.80	Joback Method
cpg	248.99	J/molxK	565.08	Joback Method
cpg	258.92	J/molxK	603.36	Joback Method

cpg	268.15	J/mol×K	641.64	Joback Method
cpg	276.74	J/mol×K	679.92	Joback Method
cpg	284.70	J/mol×K	718.20	Joback Method
dvisc	0.0031137	Paxs	263.70	Joback Method
dvisc	0.0015886	Paxs	301.17	Joback Method
dvisc	0.0009407	Paxs	338.64	Joback Method
dvisc	0.0006183	Paxs	376.11	Joback Method
dvisc	0.0004385	Paxs	413.58	Joback Method
dvisc	0.0003293	Paxs	451.05	Joback Method
dvisc	0.0002584	Paxs	488.52	Joback Method

Correlations

Information	Value
Property code	pvap
Equation	$\ln(P_{vp}) = A + B/(T + C)$
Coeff. A	1.29397e+01
Coeff. B	-3.54030e+03
Coeff. C	-7.64060e+01
Temperature range (K), min.	356.23
Temperature range (K), max.	540.51

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C23063367&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/ci9903071
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
hvac:	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

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