BENZENE, 1-(CHLOROMETHYL)-2,4-DIMETHYL-

Other names: 1,3-Dimethyl-4-(chloromethyl)benzene
1-(Chloromethyl)-2,4-dimethylbenzene
2,4-Dimethyl-1-(chloromethyl)benzene
4-(Chloromethyl)-m-xylene

Inchi: InChI=1S/C9H11Cl/c1-7-3-4-9(6-10)8(2)5-7/h3-5H,6H2,1-2H3

InchiKey: BETNPSBTDMBHCZ-UHFFFAOYSA-N

Formula: C9H11Cl

SMILES: Cc1ccc(CCl)c(C)c1

Mol. weight [g/mol]: 154.64

CAS: 824-55-5

Physical Properties

Property code	Value	Unit	Source
af	0.4010		Cheméo Relay (1.0)
gf	106.12	kJ/mol	Joback Method
hf	-53.22	kJ/mol	Cheméo Relay (1.0)
hfus	16.53	kJ/mol	Joback Method
hvap	56.23	kJ/mol	Cheméo Relay (1.0)
ie	8.61	eV	Cheméo Relay (1.0)
log10ws	-3.51		Cheméo Relay (1.0)
logp	3.042		Crippen Method
mcvol	126.150	ml/mol	McGowan Method
pc	3025.61	kPa	Joback Method
rinpol	1207.00		NIST Webbook
rinpol	1208.00		NIST Webbook
rinpol	1207.00		NIST Webbook
tb	497.26	K	Cheméo Relay (1.0)
tc	710.73	K	Cheméo Relay (1.0)
tf	284.41	K	Cheméo Relay (1.0)
vc	0.459	m3/kmol	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source

cpg	243.19	J/mol×K	479.39	Joback Method
cpg	255.67	J/mol×K	515.44	Joback Method
cpg	267.48	J/mol×K	551.49	Joback Method
cpg	278.64	J/mol×K	587.55	Joback Method
cpg	289.18	J/mol×K	623.60	Joback Method
cpg	299.10	J/mol×K	659.65	Joback Method
cpg	308.45	J/mol×K	695.70	Joback Method
dvisc	0.0017313	Pa×s	272.57	Joback Method
dvisc	0.0010303	Pa×s	307.04	Joback Method
dvisc	0.0006809	Pa×s	341.51	Joback Method
dvisc	0.0004855	Pa×s	375.98	Joback Method
dvisc	0.0003664	Pa×s	410.45	Joback Method
dvisc	0.0002888	Pa×s	444.92	Joback Method
dvisc	0.0002356	Pa×s	479.39	Joback Method

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.43358e+01
Coeff. B	-3.98863e+03
Coeff. C	-7.69950e+01
Temperature range (K), min.	360.92
Temperature range (K), max.	518.98

Sources

The Yaws Handbook of Vapor Pressure: https://www.sciencedirect.com/book/9780128029992/the-yaws-handbook-of-vapor-pressure
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C824555&Units=SI
Joback Method: https://en.wikipedia.org/wiki/Joback_method
McGowan Method: http://link.springer.com/article/10.1007/BF02311772
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws
Cheméo Relay (1.0):
Cheméo Relay (1.0, beta):

Legend

af:	Acentric Factor
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
ie:	Ionization energy
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