2,5-Dimethylbenzyl chloride

Other names:	1,4-Dimethyl-2-(chloromethyl)benzene
	1-Chloromethyl-2,5-dimethylbenzene
	2-Chloromethyl-p-xylene
	Benzene, 2-(chloromethyl)-1,4-dimethyl-
Inchi:	InChI=1S/C9H11Cl/c1-7-3-4-8(2)9(5-7)6-10/h3-5H,6H2,1-2H3
InchiKey:	PECXPZGFZFGDRD-UHFFFAOYSA-N
Formula:	C9H11Cl
SMILES:	Cc1ccc(C)c(CCl)c1
Mol. weight [g/mol]:	154.64
CAS:	824-45-3

Physical Properties

Property code	Value	Unit	Source
gf	106.12	kJ/mol	Joback Method
hf	-31.24	kJ/mol	Joback Method
hfus	16.53	kJ/mol	Joback Method
hvap	43.61	kJ/mol	Joback Method
log10ws	-3.46		Crippen Method
logp	3.042		Crippen Method
mcvol	126.150	ml/mol	McGowan Method
pc	3025.61	kPa	Joback Method
rinpol	1231.00		NIST Webbook
rinpol	1228.00		NIST Webbook
tb	496.70	K	NIST Webbook
tc	695.70	K	Joback Method
tf	272.57	K	Joback Method
vc	0.480	m3/kmol	Joback Method

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	1.42619e+01
Coeff. B	-4.02603e+03
Coeff. C	-7.92190e+01
Temperature range (K), min.	367.32
Temperature range (K), max.	529.03

Sources

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

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C824453&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
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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