Benzene, (chloromethyl)pentamethyl-

Other names:	(Chloromethyl)pentamethylbenzene
	2,3,4,5,6-Pentamethylbenzyl chloride
	Pentamethyl(chloromethyl)benzene
	Pentamethylbenzyl chloride
Inchi:	InChI=1S/C12H17Cl/c1-7-8(2)10(4)12(6-13)11(5)9(7)3/h6H2,1-5H3
InchiKey:	CXUAEBDTJFKMBV-UHFFFAOYSA-N
Formula:	C12H17Cl
SMILES:	Cc1c(C)c(C)c(CCl)c(C)c1C
Mol. weight [g/mol]:	196.72
CAS:	484-65-1

Physical Properties

Property code	Value	Unit	Source
gf	102.49	kJ/mol	Joback Method
hf	-127.57	kJ/mol	Joback Method
hfus	23.13	kJ/mol	Joback Method
hvap	52.28	kJ/mol	Joback Method
log10ws	-4.88		Crippen Method
logp	3.967		Crippen Method
mcvol	168.420	ml/mol	McGowan Method
pc	2161.32	kPa	Joback Method
tb	562.97	K	Joback Method
tc	772.55	K	Joback Method
tf	343.94	K	Joback Method
vc	0.648	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	376.32	J/mol×K	562.97	Joback Method
cpg	442.37	J/mol×K	737.62	Joback Method
cpg	430.44	J/mol×K	702.69	Joback Method
cpg	417.88	J/mol×K	667.76	Joback Method
cpg	404.68	J/mol×K	632.83	Joback Method

cpg	390.83	J/mol×K	597.90	Joback Method
cpg	453.68	J/mol×K	772.55	Joback Method
dvisc	0.0001861	Pa×s	562.97	Joback Method
dvisc	0.0002208	Pa×s	526.47	Joback Method
dvisc	0.0002688	Pa×s	489.96	Joback Method
dvisc	0.0003376	Pa×s	453.46	Joback Method
dvisc	0.0004415	Pa×s	416.95	Joback Method
dvisc	0.0006077	Pa×s	380.44	Joback Method
dvisc	0.0008953	Pa×s	343.94	Joback Method

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.18215e+01
Coeff. B	-3.40331e+03
Coeff. C	-8.29300e+01
Temperature range (K), min.	378.00
Temperature range (K), max.	605.71

Sources

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

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

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C484651&Units=SI

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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume