1-CHLORO-2-METHYL-2-PHENYLPROPANE

Other names:	(2-Chloro-1,1-dimethylethyl)benzene
	(«beta»-Chloro-«alpha»,«alpha»-dimethyl)ethylbenzene
	2-Chloromethyl-2-phenylpropane
	2-Methyl-2-phenylpropyl chloride
	Benzene, (2-chloro-1,1-dimethylethyl)-
	NSC 54159
	Neophyl chloride
	«beta»,«beta»-Dimethylphenethyl chloride
	«beta»-Chloro-tert-butylbenzene
Inchi:	InChI=1S/C10H13Cl/c1-10(2,8-11)9-6-4-3-5-7-9/h3-7H,8H2,1-2H3
InchiKey:	DNXXUUPUQXSUFH-UHFFFAOYSA-N
Formula:	C10H13Cl
SMILES:	CC(C)(CCl)c1ccccc1
Mol. weight [g/mol]:	168.67
CAS:	515-40-2

Physical Properties

Property code	Value	Unit	Source
af	0.3202		Cheméo Relay (1.0)
hf	-59.83	kJ/mol	Cheméo Relay (1.0)
hfus	12.48	kJ/mol	Joback Method
hvap	54.72	kJ/mol	Cheméo Relay (1.0)
ie	8.94	eV	Cheméo Relay (1.0)
log10ws	-4.09		Cheméo Relay (1.0)
logp	3.203		Crippen Method
mcvol	140.240	ml/mol	McGowan Method
pc	2875.03	kPa	Joback Method
tb	491.29	K	Cheméo Relay (1.0)
tc	720.98	K	Cheméo Relay (1.0)
tf	260.86	K	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source

cpg	288.27	J/mol×K	489.08	Joback Method
cpg	303.93	J/mol×K	526.55	Joback Method
cpg	318.46	J/mol×K	564.01	Joback Method
cpg	331.92	J/mol×K	601.48	Joback Method
cpg	344.37	J/mol×K	638.94	Joback Method
cpg	355.89	J/mol×K	676.41	Joback Method
cpg	366.54	J/mol×K	713.87	Joback Method
dvisc	0.0049005	Pa×s	261.22	Joback Method
dvisc	0.0021481	Pa×s	299.20	Joback Method
dvisc	0.0011339	Pa×s	337.17	Joback Method
dvisc	0.0006812	Pa×s	375.15	Joback Method
dvisc	0.0004494	Pa×s	413.13	Joback Method
dvisc	0.0003180	Pa×s	451.10	Joback Method
dvisc	0.0002374	Pa×s	489.08	Joback Method

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.42756e+01
Coeff. B	-4.02631e+03
Coeff. C	-7.90800e+01
Temperature range (K), min.	366.92
Temperature range (K), max.	528.24

Sources

Cheméo Relay (1.0, beta):

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=C515402&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):

Legend

af:	Acentric Factor
cpg:	Ideal gas heat capacity
dvisc:	Dynamic viscosity
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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point