Benzene, (2-chloro-1-methylethyl)-

Other names:	(2-Chloro-1-methylethyl)benzene
	(«beta»-Chloroisopropyl)benzene
	(Â«betaÂ»-Chloroisopropyl)benzene
	1-Chloro-2-phenylpropane
	Benzene, [1-(chloromethyl)ethyl]
	Cumene, «beta»-chloro-
	Cumene, Â«betaÂ»-chloro-
	«beta»-Chlorocumene
	Â«betaÂ»-Chlorocumene
Inchi:	InChI=1S/C9H11Cl/c1-8(7-10)9-5-3-2-4-6-9/h2-6,8H,7H2,1H3
InchiKey:	SXVRSCIZJBGJGB-UHFFFAOYSA-N
Formula:	C9H11Cl
SMILES:	CC(CCl)c1ccccc1
Mol. weight [g/mol]:	154.64
CAS:	824-47-5

Physical Properties

Property code	Value	Unit	Source
gf	122.94	kJ/mol	Joback Method
hf	-13.58	kJ/mol	Joback Method
hfus	13.78	kJ/mol	Joback Method
hvap	41.90	kJ/mol	Joback Method
log10ws	-2.81		Crippen Method
logp	3.029		Crippen Method
mcvol	126.150	ml/mol	McGowan Method
pc	3156.17	kPa	Joback Method
rinpol	1152.00		NIST Webbook
rinpol	1131.00		NIST Webbook
rinpol	1152.00		NIST Webbook
tb	468.99	K	Joback Method
tc	687.77	K	Joback Method
tf	232.53	K	Joback Method
vc	0.474	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	242.63	J/mol×K	468.99	Joback Method
cpg	303.30	J/mol×K	651.31	Joback Method
cpg	292.74	J/mol×K	614.85	Joback Method
cpg	281.43	J/mol×K	578.38	Joback Method
cpg	269.33	J/mol×K	541.92	Joback Method
cpg	256.41	J/mol×K	505.45	Joback Method
cpg	313.15	J/mol×K	687.77	Joback Method
dvisc	0.0002441	Pa×s	468.99	Joback Method
dvisc	0.0003211	Pa×s	429.58	Joback Method
dvisc	0.0004463	Pa×s	390.17	Joback Method
dvisc	0.0006679	Pa×s	350.76	Joback Method
dvisc	0.0011072	Pa×s	311.35	Joback Method
dvisc	0.0021248	Pa×s	271.94	Joback Method
dvisc	0.0050859	Pa×s	232.53	Joback Method

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.38272e+01
Coeff. B	-3.79701e+03
Coeff. C	-7.51370e+01
Temperature range (K), min.	355.57
Temperature range (K), max.	521.02

Sources

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=C824475&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

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