Benzene, 1-(chloromethyl)-2-ethyl

Inchi: InChI=1S/C9H11Cl/c1-2-8-5-3-4-6-9(8)7-10/h3-6H,2,7H2,1H3
InchiKey: IYRCFBNKBGBMIT-UHFFFAOYSA-N
Formula: C9H11Cl
SMILES: CCc1ccccc1CCl
Mol. weight [g/mol]: 154.64

Physical Properties

Property code	Value	Unit	Source
gf	115.75	kJ/mol	Joback Method
hf	-19.77	kJ/mol	Joback Method
hfus	16.92	kJ/mol	Joback Method
hvap	42.95	kJ/mol	Joback Method
log10ws	-3.31		Crippen Method
logp	2.988		Crippen Method
mcvol	126.150	ml/mol	McGowan Method
pc	3076.16	kPa	Joback Method
rinpol	1166.00		NIST Webbook
tb	474.41	K	Joback Method
tc	689.41	K	Joback Method
tf	260.05	K	Joback Method
vc	0.480	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	242.90	J/mol×K	474.41	Joback Method
cpg	255.82	J/mol×K	510.24	Joback Method
cpg	267.99	J/mol×K	546.08	Joback Method
cpg	279.46	J/mol×K	581.91	Joback Method
cpg	290.24	J/mol×K	617.74	Joback Method
cpg	300.36	J/mol×K	653.58	Joback Method
cpg	309.86	J/mol×K	689.41	Joback Method
dvisc	0.0023979	Pa×s	260.05	Joback Method
dvisc	0.0013040	Pa×s	295.78	Joback Method

dvisc	0.0008087	Pa×s	331.50	Joback Method
dvisc	0.0005504	Pa×s	367.23	Joback Method
dvisc	0.0004010	Pa×s	402.96	Joback Method
dvisc	0.0003076	Pa×s	438.68	Joback Method
dvisc	0.0002456	Pa×s	474.41	Joback Method

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=R129667&Units=SI
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
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume