

Benzene, (1-chloro-1-ethylpropyl)

Inchi:	InChI=1S/C11H15Cl/c1-3-11(12,4-2)10-8-6-5-7-9-10/h5-9H,3-4H2,1-2H3
InchiKey:	LHMUUYGTNILHKI-UHFFFAOYSA-N
Formula:	C11H15Cl
SMILES:	CCC(Cl)(CC)c1ccccc1
Mol. weight [g/mol]:	182.69

Physical Properties

Property code	Value	Unit	Source
gf	145.06	kJ/mol	Joback Method
hf	-58.33	kJ/mol	Joback Method
hfus	15.07	kJ/mol	Joback Method
hvap	45.45	kJ/mol	Joback Method
log10ws	-3.85		Crippen Method
logp	3.941		Crippen Method
mcvol	154.330	ml/mol	McGowan Method
pc	2600.43	kPa	Joback Method
rinqol	1259.00		NIST Webbook
tb	511.96	K	Joback Method
tc	732.97	K	Joback Method
tf	272.49	K	Joback Method
vc	0.582	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	333.04	J/molxK	511.96	Joback Method
cpg	349.50	J/molxK	548.80	Joback Method
cpg	364.81	J/molxK	585.63	Joback Method
cpg	379.03	J/molxK	622.47	Joback Method
cpg	392.23	J/molxK	659.30	Joback Method
cpg	404.48	J/molxK	696.14	Joback Method
cpg	415.84	J/molxK	732.97	Joback Method
dvisc	0.0046976	Paxs	272.49	Joback Method
dvisc	0.0020281	Paxs	312.40	Joback Method

dvisc	0.0010592	Paxs	352.31	Joback Method
dvisc	0.0006313	Paxs	392.23	Joback Method
dvisc	0.0004140	Paxs	432.14	Joback Method
dvisc	0.0002916	Paxs	472.05	Joback Method
dvisc	0.0002169	Paxs	511.96	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R131754&Units=SI
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
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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