

Benzene, (3-chloro-1-ethylpropyl)

Inchi:	InChI=1S/C11H15Cl/c1-2-10(8-9-12)11-6-4-3-5-7-11/h3-7,10H,2,8-9H2,1H3
InchiKey:	JYGDHUUHLWCXBCF-UHFFFAOYSA-N
Formula:	C11H15Cl
SMILES:	CCC(CCCl)c1ccccc1
Mol. weight [g/mol]:	182.69

Physical Properties

Property code	Value	Unit	Source
gf	139.78	kJ/mol	Joback Method
hf	-54.86	kJ/mol	Joback Method
hfus	18.96	kJ/mol	Joback Method
hvap	46.35	kJ/mol	Joback Method
log10ws	-3.65		Crippen Method
logp	3.809		Crippen Method
mcvol	154.330	ml/mol	McGowan Method
pc	2571.50	kPa	Joback Method
rinsol	1310.00		NIST Webbook
tb	514.75	K	Joback Method
tc	726.81	K	Joback Method
tf	255.07	K	Joback Method
vc	0.587	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	330.19	J/molxK	514.75	Joback Method
cpg	345.85	J/molxK	550.09	Joback Method
cpg	360.58	J/molxK	585.44	Joback Method
cpg	374.40	J/molxK	620.78	Joback Method
cpg	387.37	J/molxK	656.12	Joback Method
cpg	399.52	J/molxK	691.46	Joback Method
cpg	410.90	J/molxK	726.81	Joback Method
dvisc	0.0049594	Paxs	255.07	Joback Method
dvisc	0.0020092	Paxs	298.35	Joback Method

dvisc	0.0010234	Paxs	341.63	Joback Method
dvisc	0.0006066	Paxs	384.91	Joback Method
dvisc	0.0003997	Paxs	428.19	Joback Method
dvisc	0.0002843	Paxs	471.47	Joback Method
dvisc	0.0002142	Paxs	514.75	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R132099&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
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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