

# threo-Benzene, (2-chloro-1-ethylpropyl)

<b>Inchi:</b>	InChI=1S/C11H15Cl/c1-3-11(9(2)12)10-7-5-4-6-8-10/h4-9,11H,3H2,1-2H3/t9-,11+/m0/s1
<b>InchiKey:</b>	BLLBIQCCXSGGPP-GXSJLCMTSA-N
<b>Formula:</b>	C11H15Cl
<b>SMILES:</b>	CCC(c1ccccc1)C(C)Cl
<b>Mol. weight [g/mol]:</b>	182.69

## Physical Properties

Property code	Value	Unit	Source
gf	137.34	kJ/mol	Joback Method
hf	-60.14	kJ/mol	Joback Method
hfus	15.44	kJ/mol	Joback Method
hvap	45.97	kJ/mol	Joback Method
log10ws	-3.76		Crippen Method
logp	3.808		Crippen Method
mcvol	154.330	ml/mol	McGowan Method
pc	2592.49	kPa	Joback Method
rinsol	1282.00		NIST Webbook
tb	514.31	K	Joback Method
tc	731.21	K	Joback Method
tf	240.07	K	Joback Method
vc	0.581	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	330.44	J/molxK	514.31	Joback Method
cpg	401.43	J/molxK	695.06	Joback Method
cpg	389.04	J/molxK	658.91	Joback Method
cpg	375.79	J/molxK	622.76	Joback Method
cpg	361.64	J/molxK	586.61	Joback Method
cpg	346.53	J/molxK	550.46	Joback Method
cpg	413.00	J/molxK	731.21	Joback Method
dvisc	0.0002021	Paxs	514.31	Joback Method
dvisc	0.0002752	Paxs	468.60	Joback Method

dvisc	0.0004005	Paxs	422.90	Joback Method
dvisc	0.0006382	Paxs	377.19	Joback Method
dvisc	0.0011567	Paxs	331.48	Joback Method
dvisc	0.0025354	Paxs	285.78	Joback Method
dvisc	0.0074933	Paxs	240.07	Joback Method

## Sources

<b>Joback Method:</b>	<a href="https://en.wikipedia.org/wiki/Joback_method">https://en.wikipedia.org/wiki/Joback_method</a>
<b>McGowan Method:</b>	<a href="http://link.springer.com/article/10.1007/BF02311772">http://link.springer.com/article/10.1007/BF02311772</a>
<b>NIST Webbook:</b>	<a href="http://webbook.nist.gov/cgi/cbook.cgi?ID=R132282&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=R132282&amp;Units=SI</a>
<b>Crippen Method:</b>	<a href="http://pubs.acs.org/doi/abs/10.1021/ci9903071">http://pubs.acs.org/doi/abs/10.1021/ci9903071</a>
<b>Crippen Method:</b>	<a href="https://www.chemeo.com/doc/models/crippen_log10ws">https://www.chemeo.com/doc/models/crippen_log10ws</a>

## Legend

<b>cpg:</b>	Ideal gas heat capacity
<b>dvisc:</b>	Dynamic viscosity
<b>gf:</b>	Standard Gibbs free energy of formation
<b>hf:</b>	Enthalpy of formation at standard conditions
<b>hfus:</b>	Enthalpy of fusion at standard conditions
<b>hvap:</b>	Enthalpy of vaporization at standard conditions
<b>log10ws:</b>	Log10 of Water solubility in mol/l
<b>logp:</b>	Octanol/Water partition coefficient
<b>mccvol:</b>	McGowan's characteristic volume
<b>pc:</b>	Critical Pressure
<b>rinpol:</b>	Non-polar retention indices
<b>tb:</b>	Normal Boiling Point Temperature
<b>tc:</b>	Critical Temperature
<b>tf:</b>	Normal melting (fusion) point
<b>vc:</b>	Critical Volume

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