

Benzene, [1-(chloromethyl)-2-methylpropyl]

Inchi:	InChI=1S/C11H15Cl/c1-9(2)11(8-12)10-6-4-3-5-7-10/h3-7,9,11H,8H2,1-2H3
InchiKey:	AXBNMPTWUWEFAH-UHFFFAOYSA-N
Formula:	C11H15Cl
SMILES:	CC(C)C(CCl)c1ccccc1
Mol. weight [g/mol]:	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	-3.41		Crippen Method
logp	3.665		Crippen Method
mcvol	154.330	ml/mol	McGowan Method
pc	2592.49	kPa	Joback Method
tb	514.31	K	Joback Method
tc	731.21	K	Joback Method
tf	240.07	K	Joback Method
vc	0.581	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	330.44	J/molxK	514.31	Joback Method
cpg	346.53	J/molxK	550.46	Joback Method
cpg	361.64	J/molxK	586.61	Joback Method
cpg	375.79	J/molxK	622.76	Joback Method
cpg	389.04	J/molxK	658.91	Joback Method
cpg	401.43	J/molxK	695.06	Joback Method
cpg	413.00	J/molxK	731.21	Joback Method
dvisc	0.0074933	Paxs	240.07	Joback Method
dvisc	0.0025354	Paxs	285.78	Joback Method
dvisc	0.0011567	Paxs	331.48	Joback Method

dvisc	0.0006382	Paxs	377.19	Joback Method
dvisc	0.0004005	Paxs	422.90	Joback Method
dvisc	0.0002752	Paxs	468.60	Joback Method
dvisc	0.0002021	Paxs	514.31	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=R131838&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071

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
hvac:	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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

Latest version available from:

<https://www.chemeo.com/cid/77-881-9/Benzene-1-chloromethyl-2-methylpropyl.pdf>

Generated by Cheméo on 2024-04-26 19:48:07.255559497 +0000 UTC m=+16450136.176136810.

Cheméo (<https://www.chemeo.com>) is the biggest free database of chemical and physical data for the process industry.