

Benzene, 1,3,5-tris-(chloromethyl)

Inchi:	InChI=1S/C9H9Cl3/c10-4-7-1-8(5-11)3-9(2-7)6-12/h1-3H,4-6H2
InchiKey:	PJKMOHIGRNELRP-UHFFFAOYSA-N
Formula:	C9H9Cl3
SMILES:	ClCc1cc(CCl)cc(CCl)c1
Mol. weight [g/mol]:	223.53

Physical Properties

Property code	Value	Unit	Source
gf	82.26	kJ/mol	Joback Method
hf	-62.72	kJ/mol	Joback Method
hfus	24.92	kJ/mol	Joback Method
hvap	52.38	kJ/mol	Joback Method
log10ws	-4.57		Crippen Method
logp	3.903		Crippen Method
mcvol	150.630	ml/mol	McGowan Method
pc	2793.56	kPa	Joback Method
rinqol	1596.00		NIST Webbook
tb	554.25	K	Joback Method
tc	780.62	K	Joback Method
tf	332.41	K	Joback Method
vc	0.579	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	292.18	J/molxK	554.25	Joback Method
cpg	303.21	J/molxK	591.98	Joback Method
cpg	313.54	J/molxK	629.71	Joback Method
cpg	323.18	J/molxK	667.44	Joback Method
cpg	332.18	J/molxK	705.17	Joback Method
cpg	340.56	J/molxK	742.90	Joback Method
cpg	348.37	J/molxK	780.62	Joback Method
dvisc	0.0016953	Paxs	332.41	Joback Method
dvisc	0.0010463	Paxs	369.38	Joback Method

dvisc	0.0007050	Paxs	406.36	Joback Method
dvisc	0.0005074	Paxs	443.33	Joback Method
dvisc	0.0003841	Paxs	480.30	Joback Method
dvisc	0.0003026	Paxs	517.28	Joback Method
dvisc	0.0002461	Paxs	554.25	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R131685&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
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

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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