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
rinpol	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	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	292.18	J/mol×K	554.25	Joback Method
cpg	340.56	J/mol×K	742.90	Joback Method
cpg	332.18	J/mol×K	705.17	Joback Method
cpg	323.18	J/mol×K	667.44	Joback Method
cpg	313.54	J/mol×K	629.71	Joback Method
cpg	303.21	J/mol×K	591.98	Joback Method
cpg	348.37	J/mol×K	780.62	Joback Method
dvisc	0.0002461	Pa×s	554.25	Joback Method
dvisc	0.0003026	Pa×s	517.28	Joback Method

dvisc	0.0003841	Pa×s	480.30	Joback Method
dvisc	0.0005074	Pa×s	443.33	Joback Method
dvisc	0.0007050	Pa×s	406.36	Joback Method
dvisc	0.0010463	Pa×s	369.38	Joback Method
dvisc	0.0016953	Pa×s	332.41	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=R131685&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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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