

1,2-Dimethyl-3,6-bis(chloromethyl)benzene

Inchi:	InChI=1S/C10H12Cl2/c1-7-8(2)10(6-12)4-3-9(7)5-11/h3-4H,5-6H2,1-2H3
InchiKey:	SFMXDKIUJFJRIR-UHFFFAOYSA-N
Formula:	C10H12Cl2
SMILES:	Cc1c(CCl)ccc(CCl)c1C
Mol. weight [g/mol]:	203.11

Physical Properties

Property code	Value	Unit	Source
gf	92.98	kJ/mol	Joback Method
hf	-79.09	kJ/mol	Joback Method
hfus	22.92	kJ/mol	Joback Method
hvap	50.89	kJ/mol	Joback Method
log10ws	-4.49		Crippen Method
logp	3.781		Crippen Method
mcvol	152.480	ml/mol	McGowan Method
pc	2587.22	kPa	Joback Method
rinpol	1618.00		NIST Webbook
rinpol	1618.00		NIST Webbook
tb	544.68	K	Joback Method
tc	763.73	K	Joback Method
tf	326.28	K	Joback Method
vc	0.586	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	311.67	J/molxK	544.68	Joback Method
cpg	324.18	J/molxK	581.19	Joback Method
cpg	336.00	J/molxK	617.70	Joback Method
cpg	347.15	J/molxK	654.20	Joback Method
cpg	357.67	J/molxK	690.71	Joback Method
cpg	367.56	J/molxK	727.22	Joback Method
cpg	376.86	J/molxK	763.73	Joback Method
dvisc	0.0013745	Paxs	326.28	Joback Method

dvisc	0.0008734	Paxs	362.68	Joback Method
dvisc	0.0006028	Paxs	399.08	Joback Method
dvisc	0.0004426	Paxs	435.48	Joback Method
dvisc	0.0003409	Paxs	471.88	Joback Method
dvisc	0.0002726	Paxs	508.28	Joback Method
dvisc	0.0002245	Paxs	544.68	Joback Method

Sources

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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R520199&Units=SI

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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