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/mol×K	544.68	Joback Method
cpg	324.18	J/mol×K	581.19	Joback Method
cpg	336.00	J/mol×K	617.70	Joback Method
cpg	347.15	J/mol×K	654.20	Joback Method
cpg	357.67	J/mol×K	690.71	Joback Method
cpg	367.56	J/mol×K	727.22	Joback Method
cpg	376.86	J/mol×K	763.73	Joback Method
dvisc	0.0013745	Pa×s	326.28	Joback Method

dvisc	0.0008734	Pa×s	362.68	Joback Method
dvisc	0.0006028	Pa×s	399.08	Joback Method
dvisc	0.0004426	Pa×s	435.48	Joback Method
dvisc	0.0003409	Pa×s	471.88	Joback Method
dvisc	0.0002726	Pa×s	508.28	Joback Method
dvisc	0.0002245	Pa×s	544.68	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R520199&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
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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