2,4-Bis(chloromethyl)mesitylene

Other names: 1,3,5-Trimethyl-2,4-bis(chloromethyl)benzene
Inchi: InChI=1S/C11H14Cl2/c1-7-4-8(2)11(6-13)9(3)10(7)5-12/h4H,5-6H2,1-3H3
InchiKey: JMNDJDCLOQRCJV-UHFFFAOYSA-N
Formula: C11H14Cl2
SMILES: Cc1cc(C)c(CCl)c(C)c1CCl
Mol. weight [g/mol]: 217.13

Physical Properties

Property code	Value	Unit	Source
gf	91.77	kJ/mol	Joback Method
hf	-111.20	kJ/mol	Joback Method
hfus	25.13	kJ/mol	Joback Method
hvap	53.77	kJ/mol	Joback Method
log10ws	-4.96		Crippen Method
logp	4.089		Crippen Method
mcvol	166.570	ml/mol	McGowan Method
pc	2318.07	kPa	Joback Method
rinpol	1686.00		NIST Webbook
rinpol	1686.00		NIST Webbook
tb	572.54	K	Joback Method
tc	788.86	K	Joback Method
tf	350.07	K	Joback Method
vc	0.641	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	356.71	J/mol×K	572.54	Joback Method
cpg	369.87	J/mol×K	608.59	Joback Method
cpg	382.35	J/mol×K	644.65	Joback Method
cpg	394.17	J/mol×K	680.70	Joback Method
cpg	405.35	J/mol×K	716.75	Joback Method
cpg	415.89	J/mol×K	752.80	Joback Method
cpg	425.82	J/mol×K	788.86	Joback Method

dvisc	0.0011000	Pa×s	350.07	Joback Method
dvisc	0.0007263	Pa×s	387.15	Joback Method
dvisc	0.0005157	Pa×s	424.23	Joback Method
dvisc	0.0003868	Pa×s	461.31	Joback Method
dvisc	0.0003029	Pa×s	498.38	Joback Method
dvisc	0.0002453	Pa×s	535.46	Joback Method
dvisc	0.0002042	Pa×s	572.54	Joback Method

Sources

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=U342673&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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