2,4-DI[CHLOROMETHYL]TOLUENE

Other names: 1-Methyl-2,4-bis(chloromethyl)benzene
2,4-Di[chloromethyl]toluene
2,4-bis(chloromethyl)toluene
Benzene, 1,3-bis-(chloromethyl)-4-methyl
Benzene, 2,4-bis(chloromethyl)-1-methyl-
Inchi: InChI=1S/C9H10Cl2/c1-7-2-3-8(5-10)4-9(7)6-11/h2-4H,5-6H2,1H3
InchiKey: HKCWYAWNOIYUAS-UHFFFAOYSA-N
Formula: C9H10Cl2
SMILES: Cc1ccc(CCl)cc1CCl
Mol. weight [g/mol]: 189.09

Physical Properties

Property code	Value	Unit	Source
hfus	20.72	kJ/mol	Joback Method
ie	8.68	eV	Cheméo Relay (1.0)
logp	3.473		Crippen Method
mcvol	138.390	ml/mol	McGowan Method
rinpol	1463.00		NIST Webbook
rinpol	1399.00		NIST Webbook
rinpol	1463.00		NIST Webbook
tb	531.59	K	Cheméo Relay (1.0)
tf	332.26	K	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	268.32	J/mol×K	516.82	Joback Method
cpg	280.12	J/mol×K	553.78	Joback Method
cpg	291.23	J/mol×K	590.73	Joback Method
cpg	301.67	J/mol×K	627.69	Joback Method
cpg	311.46	J/mol×K	664.64	Joback Method
cpg	320.64	J/mol×K	701.60	Joback Method
cpg	329.23	J/mol×K	738.55	Joback Method
dvisc	0.0017596	Pa×s	302.49	Joback Method

dvisc	0.0010674	Pa×s	338.21	Joback Method
dvisc	0.0007125	Pa×s	373.93	Joback Method
dvisc	0.0005103	Pa×s	409.65	Joback Method
dvisc	0.0003855	Pa×s	445.38	Joback Method
dvisc	0.0003037	Pa×s	481.10	Joback Method
dvisc	0.0002472	Pa×s	516.82	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Cheméo Relay (1.0):	
Cheméo Relay (1.0, beta):	
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C2735059&Units=SI
Joback Method:	https://en.wikipedia.org/wiki/Joback_method

Legend

cpg:	Ideal gas heat capacity
dvisc:	Dynamic viscosity
hfus:	Enthalpy of fusion at standard conditions
ie:	Ionization energy
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tf:	Normal melting (fusion) point