di(Chloromethyl)toluene

Other names:	Benzene, 2,4-bis(chloromethyl)-1-methyl-
	2,4-Di[chloromethyl]toluene
	1-Methyl-2,4-bis(chloromethyl)benzene
	Benzene, 1,3-bis-(chloromethyl)-4-methyl
	2,4-bis(chloromethyl)toluene
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]:	189.08
CAS:	2735-05-9

Physical Properties

Property code	Value	Unit	Source
gf	94.19	kJ/mol	Joback Method
hf	-46.98	kJ/mol	Joback Method
hfus	20.72	kJ/mol	Joback Method
hvap	48.00	kJ/mol	Joback Method
log10ws	-4.01		Crippen Method
logp	3.473		Crippen Method
mcvol	138.390	ml/mol	McGowan Method
pc	2906.11	kPa	Joback Method
rinpol	1463.00		NIST Webbook
rinpol	1463.00		NIST Webbook
rinpol	1399.00		NIST Webbook
tb	516.82	K	Joback Method
tc	738.55	K	Joback Method
tf	302.49	K	Joback Method
vc	0.529	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	268.32	J/mol×K	516.82	Joback Method

cpg	320.64	J/mol×K	701.60	Joback Method
cpg	311.46	J/mol×K	664.64	Joback Method
cpg	301.67	J/mol×K	627.69	Joback Method
cpg	291.23	J/mol×K	590.73	Joback Method
cpg	280.12	J/mol×K	553.78	Joback Method
cpg	329.23	J/mol×K	738.55	Joback Method
dvisc	0.0002472	Pa×s	516.82	Joback Method
dvisc	0.0003037	Pa×s	481.10	Joback Method
dvisc	0.0003855	Pa×s	445.38	Joback Method
dvisc	0.0005103	Pa×s	409.66	Joback Method
dvisc	0.0007125	Pa×s	373.93	Joback Method
dvisc	0.0010674	Pa×s	338.21	Joback Method
dvisc	0.0017596	Pa×s	302.49	Joback Method

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C2735059&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