Benzene, 2,4-dichloro-5-(chloromethyl)-1,3-dimethyl

Inchi: InChI=1S/C9H9Cl3/c1-5-3-7(4-10)9(12)6(2)8(5)11/h3H,4H2,1-2H3
InchiKey: QYOZPQBWQOKBNE-UHFFFAOYSA-N
Formula: C9H9Cl3
SMILES: Cc1cc(CCl)c(Cl)c(C)c1Cl
Mol. weight [g/mol]: 223.53

Physical Properties

Property code	Value	Unit	Source
gf	63.00	kJ/mol	Joback Method
hf	-85.66	kJ/mol	Joback Method
hfus	24.14	kJ/mol	Joback Method
hvap	53.71	kJ/mol	Joback Method
log10ws	-4.83		Crippen Method
logp	4.349		Crippen Method
mcvol	150.630	ml/mol	McGowan Method
pc	2707.03	kPa	Joback Method
rinpol	1525.00		NIST Webbook
tb	564.21	K	Joback Method
tc	792.76	K	Joback Method
tf	357.45	K	Joback Method
vc	0.579	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	290.38	J/mol×K	564.21	Joback Method
cpg	300.82	J/mol×K	602.30	Joback Method
cpg	310.66	J/mol×K	640.39	Joback Method
cpg	319.94	J/mol×K	678.49	Joback Method
cpg	328.66	J/mol×K	716.58	Joback Method
cpg	336.84	J/mol×K	754.67	Joback Method
cpg	344.50	J/mol×K	792.76	Joback Method
dvisc	0.0010956	Pa×s	357.45	Joback Method
dvisc	0.0007575	Pa×s	391.91	Joback Method

dvisc	0.0005559	Pa×s	426.37	Joback Method
dvisc	0.0004273	Pa×s	460.83	Joback Method
dvisc	0.0003407	Pa×s	495.29	Joback Method
dvisc	0.0002798	Pa×s	529.75	Joback Method
dvisc	0.0002353	Pa×s	564.21	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R131947&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

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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