

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
rinsol	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/molxK	564.21	Joback Method
cpg	300.82	J/molxK	602.30	Joback Method
cpg	310.66	J/molxK	640.39	Joback Method
cpg	319.94	J/molxK	678.49	Joback Method
cpg	328.66	J/molxK	716.58	Joback Method
cpg	336.84	J/molxK	754.67	Joback Method
cpg	344.50	J/molxK	792.76	Joback Method
dvisc	0.0010956	Paxs	357.45	Joback Method
dvisc	0.0007575	Paxs	391.91	Joback Method

dvisc	0.0005559	Paxs	426.37	Joback Method
dvisc	0.0004273	Paxs	460.83	Joback Method
dvisc	0.0003407	Paxs	495.29	Joback Method
dvisc	0.0002798	Paxs	529.75	Joback Method
dvisc	0.0002353	Paxs	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/ci9903071
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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