

1,2,3-Trimethyl-4-(chloromethyl)benzene

Inchi:

InChI=1S/C10H13Cl/c1-7-4-5-10(6-11)9(3)8(7)2/h4-5H,6H2,1-3H3

InchiKey:

ABGVECYGBJQQQK-UHFFFAOYSA-N

Formula:

C10H13Cl

SMILES:

Cc1ccc(CCl)c(C)c1C

Mol. weight [g/mol]:

168.66

Physical Properties

Property code	Value	Unit	Source
gf	104.91	kJ/mol	Joback Method
hf	-63.35	kJ/mol	Joback Method
hfus	18.73	kJ/mol	Joback Method
hvap	46.50	kJ/mol	Joback Method
log10ws	-3.93		Crippen Method
logp	3.351		Crippen Method
mcvol	140.240	ml/mol	McGowan Method
pc	2687.42	kPa	Joback Method
rinpol	1375.00		NIST Webbook
tb	507.25	K	Joback Method
tc	721.45	K	Joback Method
tf	296.36	K	Joback Method
vc	0.536	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	285.86	J/mol×K	507.25	Joback Method
cpg	345.43	J/mol×K	685.75	Joback Method
cpg	334.77	J/mol×K	650.05	Joback Method
cpg	323.50	J/mol×K	614.35	Joback Method
cpg	311.60	J/mol×K	578.65	Joback Method
cpg	299.06	J/mol×K	542.95	Joback Method
cpg	355.50	J/mol×K	721.45	Joback Method
dvisc	0.0002179	Pa×s	507.25	Joback Method
dvisc	0.0002639	Pa×s	472.10	Joback Method

dvisc	0.0003295	Pa×s	436.95	Joback Method
dvisc	0.0004276	Pa×s	401.81	Joback Method
dvisc	0.0005836	Pa×s	366.66	Joback Method
dvisc	0.0008506	Pa×s	331.51	Joback Method
dvisc	0.0013558	Pa×s	296.36	Joback Method

Sources

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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R520080&Units=SI

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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