Benzene, 1-(chloromethyl)-2,4,5-trimethyl-

Other names: 1,2,4-Trimethyl-5-(chloromethyl)benzene
Inchi: InChI=1S/C10H13Cl/c1-7-4-9(3)10(6-11)5-8(7)2/h4-5H,6H2,1-3H3
InchiKey: YHMFTAUOYLECGZ-UHFFFAOYSA-N
Formula: C10H13Cl
SMILES: Cc1cc(C)c(CCl)cc1C
Mol. weight [g/mol]: 168.66
CAS: 10340-77-9

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	1335.00		NIST Webbook
rinpol	1319.00		NIST Webbook
rinpol	1335.00		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

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C10340779&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