1,3,5-Trimethyl-2-(1-methylethyl)-4-(chloromethyl)

Inchi: InChI=1S/C13H19Cl/c1-8(2)13-10(4)6-9(3)12(7-14)11(13)5/h6,8H,7H2,1-5H3
InchiKey: QUTXJFLYNDTENY-UHFFFAOYSA-N
Formula: C13H19Cl
SMILES: Cc1cc(C)c(C(C)C)c(C)c1CCl
Mol. weight [g/mol]: 210.74

Physical Properties

Property code	Value	Unit	Source
gf	118.10	kJ/mol	Joback Method
hf	-142.02	kJ/mol	Joback Method
hfus	22.59	kJ/mol	Joback Method
hvap	53.45	kJ/mol	Joback Method
log10ws	-5.12		Crippen Method
logp	4.474		Crippen Method
mcvol	182.510	ml/mol	McGowan Method
pc	2021.76	kPa	Joback Method
rinpol	1602.00		NIST Webbook
rinpol	1602.00		NIST Webbook
tb	580.43	K	Joback Method
tc	790.00	K	Joback Method
tf	327.69	K	Joback Method
vc	0.699	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	424.98	J/mol×K	580.43	Joback Method
cpg	496.89	J/mol×K	755.07	Joback Method
cpg	484.02	J/mol×K	720.14	Joback Method
cpg	470.41	J/mol×K	685.21	Joback Method
cpg	456.05	J/mol×K	650.29	Joback Method
cpg	440.91	J/mol×K	615.36	Joback Method
cpg	509.04	J/mol×K	790.00	Joback Method
dvisc	0.0001656	Pa×s	580.43	Joback Method

dvisc	0.0002047	Pa×s	538.31	Joback Method
dvisc	0.0002623	Pa×s	496.18	Joback Method
dvisc	0.0003519	Pa×s	454.06	Joback Method
dvisc	0.0005014	Pa×s	411.94	Joback Method
dvisc	0.0007744	Pa×s	369.81	Joback Method
dvisc	0.0013374	Pa×s	327.69	Joback Method

Sources

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=R520253&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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