Alpha-chloroaceto-mesitylene

Inchi: InChI=1S/C11H13ClO/c1-7-4-8(2)11(9(3)5-7)10(13)6-12/h4-5H,6H2,1-3H3
InchiKey: ALJRYGQLPCEFKO-UHFFFAOYSA-N
Formula: C11H13ClO
SMILES: Cc1cc(C)c(C(=O)CCl)c(C)c1
Mol. weight [g/mol]: 196.67
CAS: 50690-12-5

Physical Properties

Property code	Value	Unit	Source
gf	-15.59	kJ/mol	Joback Method
hf	-196.57	kJ/mol	Joback Method
hfus	22.92	kJ/mol	Joback Method
hvap	55.47	kJ/mol	Joback Method
log10ws	-3.71		Crippen Method
logp	3.033		Crippen Method
mcvol	155.900	ml/mol	McGowan Method
pc	2597.78	kPa	Joback Method
tb	584.00	K	Joback Method
tc	802.99	K	Joback Method
tf	357.56	K	Joback Method
vc	0.599	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	347.40	J/mol×K	584.00	Joback Method
cpg	360.45	J/mol×K	620.50	Joback Method
cpg	372.76	J/mol×K	657.00	Joback Method
cpg	384.36	J/mol×K	693.49	Joback Method
cpg	395.27	J/mol×K	729.99	Joback Method
cpg	405.51	J/mol×K	766.49	Joback Method
cpg	415.09	J/mol×K	802.99	Joback Method
dvisc	0.0013598	Pa×s	357.56	Joback Method
dvisc	0.0008768	Pa×s	395.30	Joback Method

dvisc	0.0006103	Pa×s	433.04	Joback Method
dvisc	0.0004502	Pa×s	470.78	Joback Method
dvisc	0.0003475	Pa×s	508.52	Joback Method
dvisc	0.0002779	Pa×s	546.26	Joback Method
dvisc	0.0002288	Pa×s	584.00	Joback Method

Sources

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=C50690125&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume