1-Propanone, 2-chloro-1-(2,5-dimethylphenyl)-2-methyl-

Other names: 2-Chloro-1-(2,5-dimethylphenyl)-2-methyl-1-propanone
Inchi: InChI=1S/C12H15ClO/c1-8-5-6-9(2)10(7-8)11(14)12(3,4)13/h5-7H,1-4H3
InchiKey: VXXAHSALZMCFQS-UHFFFAOYSA-N
Formula: C12H15ClO
SMILES: Cc1ccc(C)c(C(=O)C(C)(C)Cl)c1
Mol. weight [g/mol]: 210.70
CAS: 54965-52-5

Physical Properties

Property code	Value	Unit	Source
gf	5.30	kJ/mol	Joback Method
hf	-214.49	kJ/mol	Joback Method
hfus	18.48	kJ/mol	Joback Method
hvap	55.74	kJ/mol	Joback Method
log10ws	-4.19		Crippen Method
logp	3.504		Crippen Method
mcvol	169.990	ml/mol	McGowan Method
pc	2441.06	kPa	Joback Method
tb	598.67	K	Joback Method
tc	826.03	K	Joback Method
tf	358.73	K	Joback Method
vc	0.643	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	399.09	J/mol×K	598.67	Joback Method
cpg	463.58	J/mol×K	788.14	Joback Method
cpg	452.51	J/mol×K	750.24	Joback Method
cpg	440.58	J/mol×K	712.35	Joback Method
cpg	427.74	J/mol×K	674.46	Joback Method
cpg	413.93	J/mol×K	636.56	Joback Method
cpg	473.87	J/mol×K	826.03	Joback Method
dvisc	0.0001907	Pa×s	598.67	Joback Method

dvisc	0.0002431	Pa×s	558.68	Joback Method
dvisc	0.0003216	Pa×s	518.69	Joback Method
dvisc	0.0004459	Pa×s	478.70	Joback Method
dvisc	0.0006563	Pa×s	438.71	Joback Method
dvisc	0.0010437	Pa×s	398.72	Joback Method
dvisc	0.0018407	Pa×s	358.73	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C54965525&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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume