2-Chloro-1-(4-ethylphenyl)-2-methyl-1-propanone

Other names: 2-Chloro-1-(4-ethylphenyl)-2-methyl-1-propanone
Inchi: InChI=1S/C12H15ClO/c1-4-9-5-7-10(8-6-9)11(14)12(2,3)13/h5-8H,4H2,1-3H3
InchiKey: JRCYBVHLGNUGDA-UHFFFAOYSA-N
Formula: C12H15ClO
SMILES: CCc1ccc(C(=O)C(C)(C)Cl)cc1
Mol. weight [g/mol]: 210.70

Physical Properties

Property code	Value	Unit	Source
af	0.4812		Cheméo Relay (1.0)
hf	-231.64	kJ/mol	Cheméo Relay (1.0)
hfus	18.87	kJ/mol	Joback Method
hvap	69.41	kJ/mol	Cheméo Relay (1.0)
ie	9.11	eV	Cheméo Relay (1.0)
log10ws	-4.43		Cheméo Relay (1.0)
logp	3.449		Crippen Method
mcvol	169.990	ml/mol	McGowan Method
pc	2477.65	kPa	Joback Method
tb	535.80	K	Cheméo Relay (1.0)
tc	756.18	K	Cheméo Relay (1.0)
tf	290.06	K	Cheméo Relay (1.0)
vc	0.618	m3/kmol	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	399.66	J/mol×K	593.69	Joback Method
cpg	414.77	J/mol×K	631.42	Joback Method
cpg	428.81	J/mol×K	669.14	Joback Method
cpg	441.82	J/mol×K	706.87	Joback Method
cpg	453.88	J/mol×K	744.60	Joback Method
cpg	465.06	J/mol×K	782.33	Joback Method
cpg	475.42	J/mol×K	820.05	Joback Method
dvisc	0.0023840	Pa×s	346.21	Joback Method

dvisc	0.0012574	Pa×s	387.46	Joback Method
dvisc	0.0007500	Pa×s	428.70	Joback Method
dvisc	0.0004899	Pa×s	469.95	Joback Method
dvisc	0.0003427	Pa×s	511.20	Joback Method
dvisc	0.0002529	Pa×s	552.44	Joback Method
dvisc	0.0001947	Pa×s	593.69	Joback Method

Sources

Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Cheméo Relay (1.0):	
Cheméo Relay (1.0, beta):	
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C55012696&Units=SI
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

Legend

af:	Acentric Factor
cpg:	Ideal gas heat capacity
dvisc:	Dynamic viscosity
hf:	Enthalpy of formation at standard conditions
hfus:	Enthalpy of fusion at standard conditions
hvap:	Enthalpy of vaporization at standard conditions
ie:	Ionization energy
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

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