3-Methyl-1-phenyl-2-(chloromethyl)-1-butanone

Inchi: InChI=1S/C12H15ClO/c1-9(2)11(8-13)12(14)10-6-4-3-5-7-10/h3-7,9,11H,8H2,1-2H3
InchiKey: FTOAGWYRBJEFJG-UHFFFAOYSA-N
Formula: C12H15ClO
SMILES: CC(C)C(CCl)C(=O)c1ccccc1
Mol. weight [g/mol]: 210.70

Physical Properties

Property code	Value	Unit	Source
gf	16.84	kJ/mol	Joback Method
hf	-193.36	kJ/mol	Joback Method
hfus	19.63	kJ/mol	Joback Method
hvap	54.94	kJ/mol	Joback Method
log10ws	-3.48		Crippen Method
logp	3.380		Crippen Method
mcvol	169.990	ml/mol	McGowan Method
pc	2507.52	kPa	Joback Method
rinpol	1549.00		NIST Webbook
tb	591.06	K	Joback Method
tc	812.43	K	Joback Method
tf	301.27	K	Joback Method
vc	0.642	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	397.60	J/mol×K	591.06	Joback Method
cpg	464.41	J/mol×K	775.53	Joback Method
cpg	452.90	J/mol×K	738.64	Joback Method
cpg	440.51	J/mol×K	701.74	Joback Method
cpg	427.19	J/mol×K	664.85	Joback Method
cpg	412.91	J/mol×K	627.95	Joback Method
cpg	475.09	J/mol×K	812.43	Joback Method
dvisc	0.0001938	Pa×s	591.06	Joback Method
dvisc	0.0002606	Pa×s	542.76	Joback Method

dvisc	0.0003712	Pa×s	494.46	Joback Method
dvisc	0.0005711	Pa×s	446.16	Joback Method
dvisc	0.0009752	Pa×s	397.87	Joback Method
dvisc	0.0019308	Pa×s	349.57	Joback Method
dvisc	0.0047588	Pa×s	301.27	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=R520644&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
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume