3-Methyl-1-[4-(chloromethyl)phenyl]-1-butanone

Inchi: InChI=1S/C11H13ClO/c1-8(2)7-11(13)9-3-5-10(12)6-4-9/h3-6,8H,7H2,1-2H3
InchiKey: SCNNXOZSXWBSSI-UHFFFAOYSA-N
Formula: C11H13ClO
SMILES: CC(C)CC(=O)c1ccc(Cl)cc1
Mol. weight [g/mol]: 196.67

Physical Properties

Property code	Value	Unit	Source
gf	1.23	kJ/mol	Joback Method
hf	-178.91	kJ/mol	Joback Method
hfus	20.17	kJ/mol	Joback Method
hvap	53.76	kJ/mol	Joback Method
log10ws	-3.83		Crippen Method
logp	3.569		Crippen Method
mcvol	155.900	ml/mol	McGowan Method
pc	2701.41	kPa	Joback Method
rinpol	1660.00		NIST Webbook
rinpol	1660.00		NIST Webbook
tb	573.60	K	Joback Method
tc	795.27	K	Joback Method
tf	317.52	K	Joback Method
vc	0.593	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	349.03	J/mol×K	573.60	Joback Method
cpg	362.97	J/mol×K	610.55	Joback Method
cpg	376.03	J/mol×K	647.49	Joback Method
cpg	388.24	J/mol×K	684.44	Joback Method
cpg	399.63	J/mol×K	721.38	Joback Method
cpg	410.25	J/mol×K	758.33	Joback Method
cpg	420.13	J/mol×K	795.27	Joback Method
dvisc	0.0027371	Pa×s	317.52	Joback Method

dvisc	0.0014067	Pa×s	360.20	Joback Method
dvisc	0.0008325	Pa×s	402.88	Joback Method
dvisc	0.0005448	Pa×s	445.56	Joback Method
dvisc	0.0003839	Pa×s	488.24	Joback Method
dvisc	0.0002862	Pa×s	530.92	Joback Method
dvisc	0.0002229	Pa×s	573.60	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=R520639&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