1-Phenyl-2-(chloromethyl)-1-butanone

Inchi: InChI=1S/C11H13ClO/c1-2-9(8-12)11(13)10-6-4-3-5-7-10/h3-7,9H,2,8H2,1H3
InchiKey: KYBRUOFDMKKROW-UHFFFAOYSA-N
Formula: C11H13ClO
SMILES: CCC(CCl)C(=O)c1ccccc1
Mol. weight [g/mol]: 196.67

Physical Properties

Property code	Value	Unit	Source
gf	10.86	kJ/mol	Joback Method
hf	-167.44	kJ/mol	Joback Method
hfus	20.56	kJ/mol	Joback Method
hvap	53.10	kJ/mol	Joback Method
log10ws	-3.30		Crippen Method
logp	3.134		Crippen Method
mcvol	155.900	ml/mol	McGowan Method
pc	2744.03	kPa	Joback Method
rinpol	1485.00		NIST Webbook
tb	568.62	K	Joback Method
tc	789.25	K	Joback Method
tf	305.00	K	Joback Method
vc	0.593	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	349.51	J/mol×K	568.62	Joback Method
cpg	363.75	J/mol×K	605.39	Joback Method
cpg	377.04	J/mol×K	642.16	Joback Method
cpg	389.45	J/mol×K	678.93	Joback Method
cpg	400.99	J/mol×K	715.71	Joback Method
cpg	411.73	J/mol×K	752.48	Joback Method
cpg	421.69	J/mol×K	789.25	Joback Method
dvisc	0.0037119	Pa×s	305.00	Joback Method
dvisc	0.0017402	Pa×s	348.94	Joback Method

dvisc	0.0009665	Pa×s	392.87	Joback Method
dvisc	0.0006042	Pa×s	436.81	Joback Method
dvisc	0.0004116	Pa×s	480.75	Joback Method
dvisc	0.0002990	Pa×s	524.68	Joback Method
dvisc	0.0002282	Pa×s	568.62	Joback Method

Sources

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

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=R520451&Units=SI

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