2-Phenylbutyryl chloride

Other names: «alpha»-Phenylbutyryl chloride
Benzeneacetyl chloride, «alpha»-ethyl-
Butyryl chloride, 2-phenyl-
Inchi: InChI=1S/C10H11ClO/c1-2-9(10(11)12)8-6-4-3-5-7-8/h3-7,9H,2H2,1H3
InchiKey: QGXMHCMPIAYMGT-UHFFFAOYSA-N
Formula: C10H11ClO
SMILES: CCC(C(=O)Cl)c1ccccc1
Mol. weight [g/mol]: 182.65
CAS: 36854-57-6

Physical Properties

Property code	Value	Unit	Source
gf	2.44	kJ/mol	Joback Method
hf	-146.80	kJ/mol	Joback Method
hfus	17.97	kJ/mol	Joback Method
hvap	50.87	kJ/mol	Joback Method
log10ws	-3.00		Crippen Method
logp	2.946		Crippen Method
mcvol	141.810	ml/mol	McGowan Method
pc	3042.32	kPa	Joback Method
rinpol	1032.00		NIST Webbook
tb	545.74	K	Joback Method
tc	770.42	K	Joback Method
tf	293.73	K	Joback Method
vc	0.536	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	303.48	J/mol×K	545.74	Joback Method
cpg	361.95	J/mol×K	732.97	Joback Method
cpg	351.90	J/mol×K	695.53	Joback Method
cpg	341.08	J/mol×K	658.08	Joback Method
cpg	329.43	J/mol×K	620.63	Joback Method

cpg	316.91	J/mol×K	583.19	Joback Method
cpg	371.25	J/mol×K	770.42	Joback Method
dvisc	0.0002491	Pa×s	545.74	Joback Method
dvisc	0.0003250	Pa×s	503.74	Joback Method
dvisc	0.0004450	Pa×s	461.74	Joback Method
dvisc	0.0006490	Pa×s	419.74	Joback Method
dvisc	0.0010293	Pa×s	377.73	Joback Method
dvisc	0.0018320	Pa×s	335.73	Joback Method
dvisc	0.0038452	Pa×s	293.73	Joback Method

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	417.00	K	2.00	NIST Webbook

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=C36854576&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
tbrp:	Boiling point at reduced pressure
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume