4'-(«beta»-Chloroethyl)acetophenone

Inchi: InChI=1S/C10H11ClO/c1-8(12)10-4-2-9(3-5-10)6-7-11/h2-5H,6-7H2,1H3
InchiKey: RGVUACHOYCYNMB-UHFFFAOYSA-N
Formula: C10H11ClO
SMILES: CC(=O)c1ccc(CCCl)cc1
Mol. weight [g/mol]: 182.65
CAS: 69614-95-5

Physical Properties

Property code	Value	Unit	Source
gf	-4.75	kJ/mol	Joback Method
hf	-152.99	kJ/mol	Joback Method
hfus	21.10	kJ/mol	Joback Method
hvap	51.92	kJ/mol	Joback Method
log10ws	-3.09		Crippen Method
logp	2.671		Crippen Method
mcvol	141.810	ml/mol	McGowan Method
pc	2966.57	kPa	Joback Method
tb	551.16	K	Joback Method
tc	771.98	K	Joback Method
tf	321.25	K	Joback Method
vc	0.542	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	302.67	J/mol×K	551.16	Joback Method
cpg	315.41	J/mol×K	587.96	Joback Method
cpg	327.34	J/mol×K	624.77	Joback Method
cpg	338.51	J/mol×K	661.57	Joback Method
cpg	348.95	J/mol×K	698.37	Joback Method
cpg	358.68	J/mol×K	735.18	Joback Method
cpg	367.75	J/mol×K	771.98	Joback Method
dvisc	0.0022030	Pa×s	321.25	Joback Method
dvisc	0.0012737	Pa×s	359.57	Joback Method

dvisc	0.0008183	Pa×s	397.89	Joback Method
dvisc	0.0005683	Pa×s	436.20	Joback Method
dvisc	0.0004186	Pa×s	474.52	Joback Method
dvisc	0.0003227	Pa×s	512.84	Joback Method
dvisc	0.0002580	Pa×s	551.16	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C69614955&Units=SI
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

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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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