4-Chlorobutyric acid, phenyl ester

Inchi: InChI=1S/C10H11ClO2/c11-8-4-7-10(12)13-9-5-2-1-3-6-9/h1-3,5-6H,4,7-8H2
InchiKey: PGNJLBWZQUKEHW-UHFFFAOYSA-N
Formula: C10H11ClO2
SMILES: O=C(CCCCl)Oc1ccccc1
Mol. weight [g/mol]: 198.65

Physical Properties

Property code	Value	Unit	Source
gf	-100.12	kJ/mol	Joback Method
hf	-273.74	kJ/mol	Joback Method
hfus	22.68	kJ/mol	Joback Method
hvap	53.67	kJ/mol	Joback Method
log10ws	-2.78		Crippen Method
logp	2.611		Crippen Method
mcvol	147.680	ml/mol	McGowan Method
pc	2960.12	kPa	Joback Method
rinpol	1536.00		NIST Webbook
tb	568.60	K	Joback Method
tc	785.73	K	Joback Method
tf	330.96	K	Joback Method
vc	0.560	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	326.61	J/mol×K	568.60	Joback Method
cpg	339.38	J/mol×K	604.79	Joback Method
cpg	351.36	J/mol×K	640.98	Joback Method
cpg	362.58	J/mol×K	677.16	Joback Method
cpg	373.06	J/mol×K	713.35	Joback Method
cpg	382.82	J/mol×K	749.54	Joback Method
cpg	391.88	J/mol×K	785.73	Joback Method
dvisc	0.0021527	Pa×s	330.96	Joback Method
dvisc	0.0011940	Pa×s	370.57	Joback Method

dvisc	0.0007421	Pa×s	410.17	Joback Method
dvisc	0.0005016	Pa×s	449.78	Joback Method
dvisc	0.0003612	Pa×s	489.39	Joback Method
dvisc	0.0002732	Pa×s	528.99	Joback Method
dvisc	0.0002148	Pa×s	568.60	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=U357769&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