4-Chlorobutyric acid, 4-biphenyl ester

Inchi: InChI=1S/C16H15ClO2/c17-12-4-7-16(18)19-15-10-8-14(9-11-15)13-5-2-1-3-6-13/h1-3,5
InchiKey: CTIRJFONWYTVGL-UHFFFAOYSA-N
Formula: C16H15ClO2
SMILES: O=C(CCCCl)Oc1ccc(-c2ccccc2)cc1
Mol. weight [g/mol]: 274.74

Physical Properties

Property code	Value	Unit	Source
gf	53.18	kJ/mol	Joback Method
hf	-172.52	kJ/mol	Joback Method
hfus	31.87	kJ/mol	Joback Method
hvap	69.97	kJ/mol	Joback Method
log10ws	-5.38		Crippen Method
logp	4.278		Crippen Method
mcvol	208.460	ml/mol	McGowan Method
pc	2271.90	kPa	Joback Method
rinpol	2355.00		NIST Webbook
tb	737.54	K	Joback Method
tc	973.82	K	Joback Method
tf	437.52	K	Joback Method
vc	0.788	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	543.75	J/mol×K	737.54	Joback Method
cpg	558.38	J/mol×K	776.92	Joback Method
cpg	571.82	J/mol×K	816.30	Joback Method
cpg	584.13	J/mol×K	855.68	Joback Method
cpg	595.37	J/mol×K	895.06	Joback Method
cpg	605.58	J/mol×K	934.44	Joback Method
cpg	614.84	J/mol×K	973.82	Joback Method
dvisc	0.0010146	Pa×s	437.52	Joback Method
dvisc	0.0005818	Pa×s	487.52	Joback Method

dvisc	0.0003700	Pa×s	537.53	Joback Method
dvisc	0.0002541	Pa×s	587.53	Joback Method
dvisc	0.0001852	Pa×s	637.53	Joback Method
dvisc	0.0001413	Pa×s	687.54	Joback Method
dvisc	0.0001118	Pa×s	737.54	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U360647&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
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

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