6-Chlorohexanoic acid, 4-biphenyl ester

Inchi: InChI=1S/C18H19ClO2/c19-14-6-2-5-9-18(20)21-17-12-10-16(11-13-17)15-7-3-1-4-8-15/
InchiKey: SVXWLQJIWBRKSA-UHFFFAOYSA-N
Formula: C18H19ClO2
SMILES: O=C(CCCCCCl)Oc1ccc(-c2ccccc2)cc1
Mol. weight [g/mol]: 302.80

Physical Properties

Property code	Value	Unit	Source
gf	70.02	kJ/mol	Joback Method
hf	-213.80	kJ/mol	Joback Method
hfus	37.05	kJ/mol	Joback Method
hvap	74.42	kJ/mol	Joback Method
log10ws	-6.22		Crippen Method
logp	5.058		Crippen Method
mcvol	236.640	ml/mol	McGowan Method
pc	1906.90	kPa	Joback Method
rinpol	2646.00		NIST Webbook
tb	783.30	K	Joback Method
tc	1011.53	K	Joback Method
tf	460.06	K	Joback Method
vc	0.900	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	652.33	J/mol×K	783.30	Joback Method
cpg	716.76	J/mol×K	973.49	Joback Method
cpg	706.03	J/mol×K	935.45	Joback Method
cpg	694.28	J/mol×K	897.42	Joback Method
cpg	681.45	J/mol×K	859.38	Joback Method
cpg	667.48	J/mol×K	821.34	Joback Method
cpg	726.53	J/mol×K	1011.53	Joback Method
dvisc	0.0000872	Pa×s	783.30	Joback Method
dvisc	0.0001110	Pa×s	729.43	Joback Method

dvisc	0.0001469	Pa×s	675.55	Joback Method
dvisc	0.0002040	Pa×s	621.68	Joback Method
dvisc	0.0003016	Pa×s	567.81	Joback Method
dvisc	0.0004838	Pa×s	513.93	Joback Method
dvisc	0.0008671	Pa×s	460.06	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=U354733&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

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