

4-Chlorobutyric acid, 2-biphenyl ester

Inchi:	InChI=1S/C16H15ClO2/c17-12-6-11-16(18)19-15-10-5-4-9-14(15)13-7-2-1-3-8-13/h1-5,7
InchiKey:	LBYNLGXLCDTASA-UHFFFAOYSA-N
Formula:	C16H15ClO2
SMILES:	O=C(CCCCl)Oc1ccccc1-c1ccccc1
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
rinpola	2091.00		NIST Webbook
tb	737.54	K	Joback Method
tc	973.82	K	Joback Method
tf	437.52	K	Joback Method
vc	0.788	m ³ /kmol	Joback Method

Temperature Dependent Properties

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

dvisc	0.0003700	Paxs	537.53	Joback Method
dvisc	0.0002541	Paxs	587.53	Joback Method
dvisc	0.0001852	Paxs	637.53	Joback Method
dvisc	0.0001413	Paxs	687.54	Joback Method
dvisc	0.0001118	Paxs	737.54	Joback Method

Sources

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=U357390&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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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