Carbonic acid, 2-chloroethyl 4-benzyloxyphenyl ester

Inchi: InChI=1S/C16H15ClO4/c17-10-11-19-16(18)21-15-8-6-14(7-9-15)20-12-13-4-2-1-3-5-13/

InchiKey: WAYYAWJZDCWAHE-UHFFFAOYSA-N

Formula: C16H15ClO4

SMILES: O=C(OCCCl)Oc1ccc(OCc2ccccc2)cc1

Mol. weight [g/mol]: 306.74

Physical Properties

Property code	Value	Unit	Source
gf	-156.82	kJ/mol	Joback Method
hf	-436.96	kJ/mol	Joback Method
hfus	34.25	kJ/mol	Joback Method
hvap	74.78	kJ/mol	Joback Method
log10ws	-4.65		Crippen Method
logp	4.020		Crippen Method
mcvol	220.200	ml/mol	McGowan Method
pc	2200.01	kPa	Joback Method
rinpol	2467.00		NIST Webbook
rinpol	2467.00		NIST Webbook
tb	782.38	K	Joback Method
tc	1012.63	K	Joback Method
tf	481.98	K	Joback Method
vc	0.825	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	595.82	J/mol×K	782.38	Joback Method
cpg	609.48	J/mol×K	820.75	Joback Method
cpg	621.92	J/mol×K	859.13	Joback Method
cpg	633.17	J/mol×K	897.50	Joback Method
cpg	643.25	J/mol×K	935.88	Joback Method
cpg	652.15	J/mol×K	974.25	Joback Method
cpg	659.91	J/mol×K	1012.63	Joback Method
dvisc	0.0005268	Pa×s	481.98	Joback Method

dvisc	0.0003161	Pa×s	532.05	Joback Method
dvisc	0.0002071	Pa×s	582.11	Joback Method
dvisc	0.0001451	Pa×s	632.18	Joback Method
dvisc	0.0001071	Pa×s	682.25	Joback Method
dvisc	0.0000824	Pa×s	732.31	Joback Method
dvisc	0.0000655	Pa×s	782.38	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U357891&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