Carbonic acid, 2-chloroethyl 3,5-dimethylphenyl ester

Inchi: InChI=1S/C11H13ClO3/c1-8-5-9(2)7-10(6-8)15-11(13)14-4-3-12/h5-7H,3-4H2,1-2H3

InchiKey: AJEAMAFOXFXJED-UHFFFAOYSA-N

Formula: C11H13ClO3

SMILES: Cc1cc(C)cc(OC(=O)OCCCl)c1

Mol. weight [g/mol]: 228.67

Physical Properties

Property code	Value	Unit	Source
gf	-215.96	kJ/mol	Joback Method
hf	-449.54	kJ/mol	Joback Method
hfus	25.68	kJ/mol	Joback Method
hvap	59.63	kJ/mol	Joback Method
log10ws	-3.37		Crippen Method
logp	3.058		Crippen Method
mcvol	167.640	ml/mol	McGowan Method
pc	2548.19	kPa	Joback Method
rinpol	1685.00		NIST Webbook
tb	623.86	K	Joback Method
tc	836.76	K	Joback Method
tf	389.50	K	Joback Method
vc	0.634	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	396.31	J/mol×K	623.86	Joback Method
cpg	453.65	J/mol×K	801.27	Joback Method
cpg	443.61	J/mol×K	765.79	Joback Method
cpg	432.85	J/mol×K	730.31	Joback Method
cpg	421.37	J/mol×K	694.83	Joback Method
cpg	409.19	J/mol×K	659.34	Joback Method
cpg	462.98	J/mol×K	836.76	Joback Method
dvisc	0.0001501	Pa×s	623.86	Joback Method
dvisc	0.0001848	Pa×s	584.80	Joback Method

dvisc	0.0002343	Pa×s	545.74	Joback Method
dvisc	0.0003081	Pa×s	506.68	Joback Method
dvisc	0.0004241	Pa×s	467.62	Joback Method
dvisc	0.0006188	Pa×s	428.56	Joback Method
dvisc	0.0009740	Pa×s	389.50	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U357886&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

Latest version available from:
https://www.chemeo.com/cid/38-145-9/Carbonic-acid-2-chloroethyl-3-5-dimethylphenyl-ester.pdf
Generated by Cheméo on 2024-10-12 03:10:37.851158768 +0000 UTC m=+3283500.488128027.
Cheméo (https://www.chemeo.com) is the biggest free database of chemical and physical data for the process industry.