

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/molxK	623.86	Joback Method
cpg	453.65	J/molxK	801.27	Joback Method
cpg	443.61	J/molxK	765.79	Joback Method
cpg	432.85	J/molxK	730.31	Joback Method
cpg	421.37	J/molxK	694.83	Joback Method
cpg	409.19	J/molxK	659.34	Joback Method
cpg	462.98	J/molxK	836.76	Joback Method
dvisc	0.0001501	Paxs	623.86	Joback Method
dvisc	0.0001848	Paxs	584.80	Joback Method

dvisc	0.0002343	Paxs	545.74	Joback Method
dvisc	0.0003081	Paxs	506.68	Joback Method
dvisc	0.0004241	Paxs	467.62	Joback Method
dvisc	0.0006188	Paxs	428.56	Joback Method
dvisc	0.0009740	Paxs	389.50	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=U357886&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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