

Carbonic acid, 2-chloroethyl 3-methylphenyl ester

Inchi:	InChI=1S/C10H11ClO3/c1-8-3-2-4-9(7-8)14-10(12)13-6-5-11/h2-4,7H,5-6H2,1H3
InchiKey:	JQLPWUSEVZRGGN-UHFFFAOYSA-N
Formula:	C10H11ClO3
SMILES:	Cc1cccc(OC(=O)OCCCl)c1
Mol. weight [g/mol]:	214.65

Physical Properties

Property code	Value	Unit	Source
gf	-214.75	kJ/mol	Joback Method
hf	-417.43	kJ/mol	Joback Method
hfus	23.48	kJ/mol	Joback Method
hvap	56.74	kJ/mol	Joback Method
log10ws	-2.90		Crippen Method
logp	2.749		Crippen Method
mcvol	153.550	ml/mol	McGowan Method
pc	2859.68	kPa	Joback Method
rinpola	1578.00		NIST Webbook
tb	596.00	K	Joback Method
tc	811.57	K	Joback Method
tf	365.71	K	Joback Method
vc	0.579	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	349.40	J/molxK	596.00	Joback Method
cpg	361.70	J/molxK	631.93	Joback Method
cpg	373.30	J/molxK	667.86	Joback Method
cpg	384.22	J/molxK	703.78	Joback Method
cpg	394.45	J/molxK	739.71	Joback Method
cpg	403.99	J/molxK	775.64	Joback Method
cpg	412.84	J/molxK	811.57	Joback Method
dvisc	0.0012484	Paxs	365.71	Joback Method
dvisc	0.0007630	Paxs	404.09	Joback Method

dvisc	0.0005079	Paxs	442.47	Joback Method
dvisc	0.0003608	Paxs	480.86	Joback Method
dvisc	0.0002696	Paxs	519.24	Joback Method
dvisc	0.0002097	Paxs	557.62	Joback Method
dvisc	0.0001684	Paxs	596.00	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U357884&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
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

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