Carbonic acid, 2,2,2-trichloroethyl phenyl ester

Inchi: InChI=1S/C9H7Cl3O3/c10-9(11,12)6-14-8(13)15-7-4-2-1-3-5-7/h1-5H,6H2
InchiKey: DCJYJZZSUQZHIG-UHFFFAOYSA-N
Formula: C9H7Cl3O3
SMILES: O=C(OCC(Cl)(Cl)Cl)Oc1ccccc1
Mol. weight [g/mol]: 269.51

Physical Properties

Property code	Value	Unit	Source
gf	-234.56	kJ/mol	Joback Method
hf	-425.55	kJ/mol	Joback Method
hfus	22.26	kJ/mol	Joback Method
hvap	61.33	kJ/mol	Joback Method
log10ws	-3.83		Crippen Method
logp	3.572		Crippen Method
mcvol	163.940	ml/mol	McGowan Method
pc	3038.96	kPa	Joback Method
rinpol	1633.00		NIST Webbook
tb	639.77	K	Joback Method
tc	879.16	K	Joback Method
tf	404.18	K	Joback Method
vc	0.610	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	353.42	J/mol×K	639.77	Joback Method
cpg	396.47	J/mol×K	839.26	Joback Method
cpg	389.50	J/mol×K	799.36	Joback Method
cpg	381.75	J/mol×K	759.47	Joback Method
cpg	373.18	J/mol×K	719.57	Joback Method
cpg	363.75	J/mol×K	679.67	Joback Method
cpg	402.70	J/mol×K	879.16	Joback Method
dvisc	0.0001432	Pa×s	639.77	Joback Method
dvisc	0.0001836	Pa×s	600.50	Joback Method

dvisc	0.0002439	Pa×s	561.24	Joback Method
dvisc	0.0003381	Pa×s	521.98	Joback Method
dvisc	0.0004942	Pa×s	482.71	Joback Method
dvisc	0.0007727	Pa×s	443.44	Joback Method
dvisc	0.0013176	Pa×s	404.18	Joback Method

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=U357896&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