Carbonic acid, 2,2,2-trichloroethyl 3-methylphenyl ester

Inchi: InChI=1S/C10H9Cl3O3/c1-7-3-2-4-8(5-7)16-9(14)15-6-10(11,12)13/h2-5H,6H2,1H3
InchiKey: RAWFKHLVIXRCQN-UHFFFAOYSA-N
Formula: C10H9Cl3O3
SMILES: Cc1cccc(OC(=O)OCC(Cl)(Cl)Cl)c1
Mol. weight [g/mol]: 283.54

Physical Properties

Property code	Value	Unit	Source
gf	-235.77	kJ/mol	Joback Method
hf	-457.66	kJ/mol	Joback Method
hfus	24.46	kJ/mol	Joback Method
hvap	64.22	kJ/mol	Joback Method
log10ws	-4.31		Crippen Method
logp	3.881		Crippen Method
mcvol	178.030	ml/mol	McGowan Method
pc	2698.60	kPa	Joback Method
rinpol	1741.00		NIST Webbook
tb	667.63	K	Joback Method
tc	902.99	K	Joback Method
tf	427.97	K	Joback Method
vc	0.665	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	399.60	J/mol×K	667.63	Joback Method
cpg	410.49	J/mol×K	706.86	Joback Method
cpg	420.50	J/mol×K	746.08	Joback Method
cpg	429.65	J/mol×K	785.31	Joback Method
cpg	437.97	J/mol×K	824.54	Joback Method
cpg	445.50	J/mol×K	863.76	Joback Method
cpg	452.28	J/mol×K	902.99	Joback Method
dvisc	0.0009868	Pa×s	427.97	Joback Method
dvisc	0.0006018	Pa×s	467.91	Joback Method

dvisc	0.0003967	Pa×s	507.86	Joback Method
dvisc	0.0002779	Pa×s	547.80	Joback Method
dvisc	0.0002043	Pa×s	587.74	Joback Method
dvisc	0.0001562	Pa×s	627.69	Joback Method
dvisc	0.0001234	Pa×s	667.63	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=U357899&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