CARBONIC ACID, T-BUTYL ESTER 2,4,5-TRICHLOROPHENYL ESTER

Other names: t-Butyl 2,4,5-trichlorophenyl carbonate
Carbonic acid, 1,1-dimethylethyl 2,4,5-trichlorophenyl ester
Inchi: InChI=1S/C11H11Cl3O3/c1-11(2,3)17-10(15)16-9-5-7(13)6(12)4-8(9)14/h4-5H,1-3H3
InchiKey: LJFPGBIHDPZHIN-UHFFFAOYSA-N
Formula: C11H11Cl3O3
SMILES: CC(C)(C)OC(=O)Oc1cc(Cl)c(Cl)cc1Cl
Mol. weight [g/mol]: 297.56

Physical Properties

Property code	Value	Unit	Source
hfus	26.27	kJ/mol	Joback Method
hvap	85.03	kJ/mol	Cheméo Relay (1.0)
log10ws	-5.44		Cheméo Relay (1.0)
logp	4.961		Crippen Method
mcvol	192.120	ml/mol	McGowan Method
tf	354.43	K	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	445.75	J/mol×K	700.47	Joback Method
cpg	457.01	J/mol×K	739.21	Joback Method
cpg	467.42	J/mol×K	777.94	Joback Method
cpg	476.99	J/mol×K	816.68	Joback Method
cpg	485.74	J/mol×K	855.42	Joback Method
cpg	493.69	J/mol×K	894.15	Joback Method
cpg	500.86	J/mol×K	932.89	Joback Method
dvisc	0.0006395	Pa×s	464.28	Joback Method
dvisc	0.0004219	Pa×s	503.64	Joback Method
dvisc	0.0002956	Pa×s	543.01	Joback Method
dvisc	0.0002174	Pa×s	582.38	Joback Method
dvisc	0.0001662	Pa×s	621.74	Joback Method
dvisc	0.0001312	Pa×s	661.11	Joback Method
dvisc	0.0001063	Pa×s	700.47	Joback Method

Sources

Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Cheméo Relay (1.0):	
Cheméo Relay (1.0, beta):	
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C16965085&Units=SI
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

Legend

cpg:	Ideal gas heat capacity
dvisc:	Dynamic viscosity
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
tf:	Normal melting (fusion) point