Carbonic acid, 2,2,2-trichloroethyl 4-benzyloxyphenyl ester

Inchi: InChI=1S/C16H13Cl3O4/c17-16(18,19)11-22-15(20)23-14-8-6-13(7-9-14)21-10-12-4-2-1

InchiKey: APNMBQJHVZLHMO-UHFFFAOYSA-N

Formula: C16H13Cl3O4

SMILES: O=C(OCC(Cl)(Cl)Cl)Oc1ccc(OCc2ccccc2)cc1

Mol. weight [g/mol]: 375.63

Physical Properties

Property code	Value	Unit	Source
gf	-177.84	kJ/mol	Joback Method
hf	-477.19	kJ/mol	Joback Method
hfus	35.23	kJ/mol	Joback Method
hvap	82.26	kJ/mol	Joback Method
log10ws	-6.06		Crippen Method
logp	5.151		Crippen Method
mcvol	244.680	ml/mol	McGowan Method
pc	2090.75	kPa	Joback Method
rinpol	2641.00		NIST Webbook
tb	854.01	K	Joback Method
tc	1100.18	K	Joback Method
tf	544.24	K	Joback Method
vc	0.911	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	641.63	J/mol×K	854.01	Joback Method
cpg	685.06	J/mol×K	1059.15	Joback Method
cpg	678.66	J/mol×K	1018.12	Joback Method
cpg	671.17	J/mol×K	977.10	Joback Method
cpg	662.54	J/mol×K	936.07	Joback Method
cpg	652.71	J/mol×K	895.04	Joback Method
cpg	690.42	J/mol×K	1100.18	Joback Method
dvisc	0.0000391	Pa×s	854.01	Joback Method
dvisc	0.0000497	Pa×s	802.38	Joback Method

dvisc	0.0000654	Pa×s	750.75	Joback Method
dvisc	0.0000896	Pa×s	699.12	Joback Method
dvisc	0.0001291	Pa×s	647.50	Joback Method
dvisc	0.0001981	Pa×s	595.87	Joback Method
dvisc	0.0003297	Pa×s	544.24	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U357906&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