Dichloroacetic acid, 4-benzyloxyphenyl ester

Inchi: InChI=1S/C15H12Cl2O3/c16-14(17)15(18)20-13-8-6-12(7-9-13)19-10-11-4-2-1-3-5-11/h1
InchiKey: BHDHMFXSIYFMCZ-UHFFFAOYSA-N
Formula: C15H12Cl2O3
SMILES: O=C(Oc1ccc(OCc2ccccc2)cc1)C(Cl)Cl
Mol. weight [g/mol]: 311.16

Physical Properties

Property code	Value	Unit	Source
gf	-74.61	kJ/mol	Joback Method
hf	-305.12	kJ/mol	Joback Method
hfus	31.14	kJ/mol	Joback Method
hvap	74.15	kJ/mol	Joback Method
log10ws	-4.93		Crippen Method
logp	3.975		Crippen Method
mcvol	212.480	ml/mol	McGowan Method
pc	2384.19	kPa	Joback Method
rinpol	2260.00		NIST Webbook
rinpol	2260.00		NIST Webbook
tb	774.07	K	Joback Method
tc	1018.23	K	Joback Method
tf	463.40	K	Joback Method
vc	0.793	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	540.32	J/mol×K	774.07	Joback Method
cpg	592.19	J/mol×K	977.54	Joback Method
cpg	584.08	J/mol×K	936.84	Joback Method
cpg	574.88	J/mol×K	896.15	Joback Method
cpg	564.55	J/mol×K	855.46	Joback Method
cpg	553.04	J/mol×K	814.76	Joback Method
cpg	599.23	J/mol×K	1018.23	Joback Method
dvisc	0.0000799	Pa×s	774.07	Joback Method

dvisc	0.0001017	Pa×s	722.29	Joback Method
dvisc	0.0001345	Pa×s	670.51	Joback Method
dvisc	0.0001862	Pa×s	618.74	Joback Method
dvisc	0.0002737	Pa×s	566.96	Joback Method
dvisc	0.0004347	Pa×s	515.18	Joback Method
dvisc	0.0007655	Pa×s	463.40	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U307591&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

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