4-(4-Hydroxybenzoyl)phenyl 2,2-dichloropropanoate

Inchi: InChI=1S/C16H12Cl2O4/c1-16(17,18)15(21)22-13-8-4-11(5-9-13)14(20)10-2-6-12(19)7-3

InchiKey: GQQYKXUULIADAL-UHFFFAOYSA-N

Formula: C16H12Cl2O4

SMILES: CC(Cl)(Cl)C(=O)Oc1ccc(C(=O)c2ccc(O)cc2)cc1

Mol. weight [g/mol]: 339.17

CAS: 116495-90-0

Physical Properties

Property code	Value	Unit	Source
gf	-239.45	kJ/mol	Joback Method
hf	-486.90	kJ/mol	Joback Method
hfus	36.04	kJ/mol	Joback Method
hvap	92.81	kJ/mol	Joback Method
log10ws	-4.62		Crippen Method
logp	3.722		Crippen Method
mcvol	228.140	ml/mol	McGowan Method
pc	2758.46	kPa	Joback Method
tb	906.23	K	Joback Method
tc	1167.27	K	Joback Method
tf	631.51	K	Joback Method
vc	0.798	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	619.65	J/mol×K	906.23	Joback Method
cpg	630.19	J/mol×K	949.74	Joback Method
cpg	640.15	J/mol×K	993.24	Joback Method
cpg	649.73	J/mol×K	1036.75	Joback Method
cpg	659.08	J/mol×K	1080.26	Joback Method
cpg	668.40	J/mol×K	1123.77	Joback Method
cpg	677.86	J/mol×K	1167.27	Joback Method
dvisc	0.0000451	Pa×s	631.51	Joback Method
dvisc	0.0000249	Pa×s	677.30	Joback Method

dvisc	0.0000148	Pa×s	723.08	Joback Method
dvisc	0.0000094	Pa×s	768.87	Joback Method
dvisc	0.0000063	Pa×s	814.66	Joback Method
dvisc	0.0000044	Pa×s	860.44	Joback Method
dvisc	0.0000032	Pa×s	906.23	Joback Method

Sources

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=C116495900&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume