2,4-Ditert-butyl-6-chlorophenyl chloroacetate

Inchi: InChI=1S/C16H22Cl2O2/c1-15(2,3)10-7-11(16(4,5)6)14(12(18)8-10)20-13(19)9-17/h7-8H
InchiKey: FNJSIWWSGGXZNM-UHFFFAOYSA-N
Formula: C16H22Cl2O2
SMILES: CC(C)(C)c1cc(Cl)c(OC(=O)CCl)c(C(C)(C)C)c1
Mol. weight [g/mol]: 317.25
CAS: 116434-87-8

Physical Properties

Property code	Value	Unit	Source
gf	-84.74	kJ/mol	Joback Method
hf	-465.23	kJ/mol	Joback Method
hfus	26.42	kJ/mol	Joback Method
hvap	70.81	kJ/mol	Joback Method
log10ws	-5.25		Crippen Method
logp	5.079		Crippen Method
mcvol	244.460	ml/mol	McGowan Method
pc	1655.15	kPa	Joback Method
tb	751.79	K	Joback Method
tc	976.27	K	Joback Method
tf	470.90	K	Joback Method
vc	0.923	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	660.46	J/mol×K	751.79	Joback Method
cpg	675.85	J/mol×K	789.20	Joback Method
cpg	690.14	J/mol×K	826.62	Joback Method
cpg	703.41	J/mol×K	864.03	Joback Method
cpg	715.72	J/mol×K	901.44	Joback Method
cpg	727.16	J/mol×K	938.86	Joback Method
cpg	737.78	J/mol×K	976.27	Joback Method
dvisc	0.0006575	Pa×s	470.90	Joback Method
dvisc	0.0003776	Pa×s	517.71	Joback Method

dvisc	0.0002377	Pa×s	564.53	Joback Method
dvisc	0.0001607	Pa×s	611.35	Joback Method
dvisc	0.0001148	Pa×s	658.16	Joback Method
dvisc	0.0000858	Pa×s	704.97	Joback Method
dvisc	0.0000665	Pa×s	751.79	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=C116434878&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