6-Chloro-2,4-di-tert-butylphenyl propionate

Inchi: InChI=1S/C17H25ClO2/c1-8-14(19)20-15-12(17(5,6)7)9-11(10-13(15)18)16(2,3)4/h9-10H
InchiKey: ZCFMAVGMRKJUOC-UHFFFAOYSA-N
Formula: C17H25ClO2
SMILES: CCC(=O)Oc1c(Cl)cc(C(C)(C)C)cc1C(C)(C)C
Mol. weight [g/mol]: 296.83
CAS: 101865-85-4

Physical Properties

Property code	Value	Unit	Source
gf	-64.39	kJ/mol	Joback Method
hf	-470.13	kJ/mol	Joback Method
hfus	24.82	kJ/mol	Joback Method
hvap	68.65	kJ/mol	Joback Method
log10ws	-5.52		Crippen Method
logp	5.250		Crippen Method
mcvol	246.310	ml/mol	McGowan Method
pc	1578.46	kPa	Joback Method
tb	737.24	K	Joback Method
tc	955.46	K	Joback Method
tf	452.25	K	Joback Method
vc	0.930	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	688.08	J/mol×K	737.24	Joback Method
cpg	762.03	J/mol×K	919.09	Joback Method
cpg	749.25	J/mol×K	882.72	Joback Method
cpg	735.53	J/mol×K	846.35	Joback Method
cpg	720.80	J/mol×K	809.98	Joback Method
cpg	705.01	J/mol×K	773.61	Joback Method
cpg	773.95	J/mol×K	955.46	Joback Method
dvisc	0.0000664	Pa×s	737.24	Joback Method
dvisc	0.0000864	Pa×s	689.74	Joback Method

dvisc	0.0001168	Pa×s	642.24	Joback Method
dvisc	0.0001657	Pa×s	594.75	Joback Method
dvisc	0.0002497	Pa×s	547.25	Joback Method
dvisc	0.0004069	Pa×s	499.75	Joback Method
dvisc	0.0007346	Pa×s	452.25	Joback Method

Sources

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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C101865854&Units=SI

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