Phthalic acid, ethyl 3,4,5-trichlorophenyl ester

Inchi: InChI=1S/C16H11Cl3O4/c1-2-22-15(20)10-5-3-4-6-11(10)16(21)23-9-7-12(17)14(19)13(
InchiKey: BDVXTPZJEIHRQQ-UHFFFAOYSA-N
Formula: C16H11Cl3O4
SMILES: CCOC(=O)c1ccccc1C(=O)Oc1cc(Cl)c(Cl)c(Cl)c1
Mol. weight [g/mol]: 373.62

Physical Properties

Property code	Value	Unit	Source
gf	-233.49	kJ/mol	Joback Method
hf	-483.21	kJ/mol	Joback Method
hfus	41.89	kJ/mol	Joback Method
hvap	89.88	kJ/mol	Joback Method
log10ws	-6.27		Crippen Method
logp	5.043		Crippen Method
mcvol	240.380	ml/mol	McGowan Method
pc	2121.68	kPa	Joback Method
rinpol	2633.00		NIST Webbook
rinpol	2633.00		NIST Webbook
tb	903.63	K	Joback Method
tc	1148.58	K	Joback Method
tf	607.08	K	Joback Method
vc	0.910	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	615.69	J/mol×K	903.63	Joback Method
cpg	624.86	J/mol×K	944.45	Joback Method
cpg	632.83	J/mol×K	985.28	Joback Method
cpg	639.63	J/mol×K	1026.10	Joback Method
cpg	645.26	J/mol×K	1066.93	Joback Method
cpg	649.73	J/mol×K	1107.75	Joback Method
cpg	653.06	J/mol×K	1148.58	Joback Method
dvisc	0.0003270	Pa×s	607.08	Joback Method

dvisc	0.0002274	Pa×s	656.50	Joback Method
dvisc	0.0001664	Pa×s	705.93	Joback Method
dvisc	0.0001268	Pa×s	755.36	Joback Method
dvisc	0.0000999	Pa×s	804.78	Joback Method
dvisc	0.0000810	Pa×s	854.20	Joback Method
dvisc	0.0000671	Pa×s	903.63	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=U357063&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
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume