Phthalic acid, 2-(3-chlorophenyl)ethyl propyl ester

Inchi: InChI=1S/C19H19ClO4/c1-2-11-23-18(21)16-8-3-4-9-17(16)19(22)24-12-10-14-6-5-7-15(

InchiKey: MHCQBYBHIRZCNH-UHFFFAOYSA-N

Formula: C19H19ClO4

SMILES: CCCOC(=O)c1ccccc1C(=O)OCCc1cccc(Cl)c1

Mol. weight [g/mol]: 346.81

Physical Properties

Property code	Value	Unit	Source
gf	-165.11	kJ/mol	Joback Method
hf	-490.71	kJ/mol	Joback Method
hfus	42.04	kJ/mol	Joback Method
hvap	86.46	kJ/mol	Joback Method
log10ws	-5.51		Crippen Method
logp	4.306		Crippen Method
mcvol	258.170	ml/mol	McGowan Method
pc	1803.09	kPa	Joback Method
rinpol	2612.00		NIST Webbook
rinpol	2612.00		NIST Webbook
tb	887.45	K	Joback Method
tc	1117.22	K	Joback Method
tf	556.01	K	Joback Method
vc	0.981	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	746.25	J/mol×K	887.45	Joback Method
cpg	797.01	J/mol×K	1078.93	Joback Method
cpg	789.24	J/mol×K	1040.63	Joback Method
cpg	780.32	J/mol×K	1002.34	Joback Method
cpg	770.20	J/mol×K	964.04	Joback Method
cpg	758.85	J/mol×K	925.75	Joback Method
cpg	803.66	J/mol×K	1117.22	Joback Method
dvisc	0.0000569	Pa×s	887.45	Joback Method

dvisc	0.0000711	Pa×s	832.21	Joback Method
dvisc	0.0000917	Pa×s	776.97	Joback Method
dvisc	0.0001228	Pa×s	721.73	Joback Method
dvisc	0.0001728	Pa×s	666.49	Joback Method
dvisc	0.0002585	Pa×s	611.25	Joback Method
dvisc	0.0004190	Pa×s	556.01	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=U377852&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
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume