Phthalic acid, 2-(4-chlorophenyl)ethyl isobutyl ester

Inchi: InChI=1S/C20H21ClO4/c1-14(2)13-25-20(23)18-6-4-3-5-17(18)19(22)24-12-11-15-7-9-16

InchiKey: HVDGPFLUBDWNIJ-UHFFFAOYSA-N

Formula: C20H21ClO4

SMILES: CC(C)COC(=O)c1ccccc1C(=O)OCCc1ccc(Cl)cc1

Mol. weight [g/mol]: 360.83

Physical Properties

Property code	Value	Unit	Source
gf	-159.13	kJ/mol	Joback Method
hf	-516.63	kJ/mol	Joback Method
hfus	41.11	kJ/mol	Joback Method
hvap	88.30	kJ/mol	Joback Method
log10ws	-5.69		Crippen Method
logp	4.552		Crippen Method
mcvol	272.260	ml/mol	McGowan Method
pc	1675.53	kPa	Joback Method
rinpol	2649.00		NIST Webbook
rinpol	2649.00		NIST Webbook
tb	909.89	K	Joback Method
tc	1140.67	K	Joback Method
tf	552.28	K	Joback Method
vc	1.030	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	803.93	J/mol×K	909.89	Joback Method
cpg	816.74	J/mol×K	948.35	Joback Method
cpg	828.22	J/mol×K	986.82	Joback Method
cpg	838.42	J/mol×K	1025.28	Joback Method
cpg	847.38	J/mol×K	1063.74	Joback Method
cpg	855.12	J/mol×K	1102.21	Joback Method
cpg	861.68	J/mol×K	1140.67	Joback Method
dvisc	0.0004114	Pa×s	552.28	Joback Method

dvisc	0.0002380	Pa×s	611.88	Joback Method
dvisc	0.0001517	Pa×s	671.48	Joback Method
dvisc	0.0001041	Pa×s	731.09	Joback Method
dvisc	0.0000756	Pa×s	790.69	Joback Method
dvisc	0.0000574	Pa×s	850.29	Joback Method
dvisc	0.0000452	Pa×s	909.89	Joback Method

Sources

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=U377837&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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