Phthalic acid, 4-chloro-2-methoxybenzyl isobutyl ester

Inchi: InChI=1S/C20H21ClO5/c1-13(2)11-25-19(22)16-6-4-5-7-17(16)20(23)26-12-14-8-9-15(21

InchiKey: NZIIXFHKKCLSPD-UHFFFAOYSA-N

Formula: C20H21ClO5

SMILES: COc1cc(Cl)ccc1COC(=O)c1ccccc1C(=O)OCC(C)C

Mol. weight [g/mol]: 376.83

Physical Properties

Property code	Value	Unit	Source
gf	-273.76	kJ/mol	Joback Method
hf	-660.32	kJ/mol	Joback Method
hfus	41.91	kJ/mol	Joback Method
hvap	91.37	kJ/mol	Joback Method
log10ws	-5.89		Crippen Method
logp	4.518		Crippen Method
mcvol	278.130	ml/mol	McGowan Method
pc	1632.49	kPa	Joback Method
rinpol	2619.00		NIST Webbook
rinpol	2619.00		NIST Webbook
tb	937.29	K	Joback Method
tc	1168.17	K	Joback Method
tf	587.03	K	Joback Method
vc	1.048	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	828.79	J/mol×K	937.29	Joback Method
cpg	840.62	J/mol×K	975.77	Joback Method
cpg	850.99	J/mol×K	1014.25	Joback Method
cpg	859.92	J/mol×K	1052.73	Joback Method
cpg	867.40	J/mol×K	1091.21	Joback Method
cpg	873.45	J/mol×K	1129.69	Joback Method
cpg	878.07	J/mol×K	1168.17	Joback Method
dvisc	0.0002596	Pa×s	587.03	Joback Method

dvisc	0.0001592	Pa×s	645.41	Joback Method
dvisc	0.0001058	Pa×s	703.78	Joback Method
dvisc	0.0000749	Pa×s	762.16	Joback Method
dvisc	0.0000557	Pa×s	820.54	Joback Method
dvisc	0.0000431	Pa×s	878.91	Joback Method
dvisc	0.0000344	Pa×s	937.29	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=U382837&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