Phthalic acid, isobutyl 2,4,6-trichlorobenzyl ester

Inchi: InChI=1S/C19H17Cl3O4/c1-11(2)9-25-18(23)13-5-3-4-6-14(13)19(24)26-10-15-16(21)7-1

InchiKey: SJRTYIOATZJLJK-UHFFFAOYSA-N

Formula: C19H17Cl3O4

SMILES: CC(C)COC(=O)c1ccccc1C(=O)OCc1c(Cl)cc(Cl)cc1Cl

Mol. weight [g/mol]: 415.69

Physical Properties

Property code	Value	Unit	Source
gf	-210.67	kJ/mol	Joback Method
hf	-550.41	kJ/mol	Joback Method
hfus	46.13	kJ/mol	Joback Method
hvap	96.17	kJ/mol	Joback Method
log10ws	-7.14		Crippen Method
logp	5.817		Crippen Method
mcvol	282.650	ml/mol	McGowan Method
pc	1664.61	kPa	Joback Method
rinpol	2708.00		NIST Webbook
rinpol	2708.00		NIST Webbook
tb	971.83	K	Joback Method
tc	1212.62	K	Joback Method
tf	625.89	K	Joback Method
vc	1.073	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	783.80	J/mol×K	971.83	Joback Method
cpg	819.16	J/mol×K	1172.49	Joback Method
cpg	814.64	J/mol×K	1132.36	Joback Method
cpg	808.87	J/mol×K	1092.22	Joback Method
cpg	801.82	J/mol×K	1052.09	Joback Method
cpg	793.47	J/mol×K	1011.96	Joback Method
cpg	822.46	J/mol×K	1212.62	Joback Method
dvisc	0.0000398	Pa×s	971.83	Joback Method

dvisc	0.0000492	Pa×s	914.17	Joback Method
dvisc	0.0000625	Pa×s	856.52	Joback Method
dvisc	0.0000821	Pa×s	798.86	Joback Method
dvisc	0.0001127	Pa×s	741.20	Joback Method
dvisc	0.0001631	Pa×s	683.55	Joback Method
dvisc	0.0002528	Pa×s	625.89	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=U382877&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