Phthalic acid, di(2,4,6-trichlorobenzyl) ester

Inchi: InChI=1S/C22H12Cl6O4/c23-11-5-17(25)15(18(26)6-11)9-31-21(29)13-3-1-2-4-14(13)22
InchiKey: XQNLRWJXCKJBAO-UHFFFAOYSA-N
Formula: C22H12Cl6O4
SMILES: O=C(OCc1c(Cl)cc(Cl)cc1Cl)c1ccccc1C(=O)OCc1c(Cl)cc(Cl)cc1Cl
Mol. weight [g/mol]: 553.05

Physical Properties

Property code	Value	Unit	Source
gf	-135.24	kJ/mol	Joback Method
hf	-452.15	kJ/mol	Joback Method
hfus	62.89	kJ/mol	Joback Method
hvap	120.65	kJ/mol	Joback Method
log10ws	-10.29		Crippen Method
logp	8.321		Crippen Method
mcvol	337.880	ml/mol	McGowan Method
pc	1511.67	kPa	Joback Method
rinpol	3434.00		NIST Webbook
tb	1194.82	K	Joback Method
tc	1470.05	K	Joback Method
tf	828.44	K	Joback Method
vc	1.286	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	868.69	J/mol×K	1194.82	Joback Method
cpg	870.65	J/mol×K	1240.69	Joback Method
cpg	871.08	J/mol×K	1286.56	Joback Method
cpg	870.01	J/mol×K	1332.44	Joback Method
cpg	867.49	J/mol×K	1378.31	Joback Method
cpg	863.57	J/mol×K	1424.18	Joback Method
cpg	858.30	J/mol×K	1470.05	Joback Method
dvisc	0.0000792	Pa×s	828.44	Joback Method
dvisc	0.0000574	Pa×s	889.50	Joback Method

dvisc	0.0000433	Pa×s	950.57	Joback Method
dvisc	0.0000339	Pa×s	1011.63	Joback Method
dvisc	0.0000272	Pa×s	1072.69	Joback Method
dvisc	0.0000224	Pa×s	1133.76	Joback Method
dvisc	0.0000188	Pa×s	1194.82	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U382889&Units=SI
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

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