Phthalic acid, di(2,4-dichlorobenzyl) ester

Inchi: InChI=1S/C22H14Cl4O4/c23-15-7-5-13(19(25)9-15)11-29-21(27)17-3-1-2-4-18(17)22(28
InchiKey: QLXUOZDLKOAJJB-UHFFFAOYSA-N
Formula: C22H14Cl4O4
SMILES: O=C(OCc1ccc(Cl)cc1Cl)c1ccccc1C(=O)OCc1ccc(Cl)cc1Cl
Mol. weight [g/mol]: 484.16

Physical Properties

Property code	Value	Unit	Source
gf	-92.12	kJ/mol	Joback Method
hf	-397.73	kJ/mol	Joback Method
hfus	55.28	kJ/mol	Joback Method
hvap	110.56	kJ/mol	Joback Method
log10ws	-8.92		Crippen Method
logp	7.014		Crippen Method
mcvol	313.400	ml/mol	McGowan Method
pc	1641.76	kPa	Joback Method
rinpol	3385.00		NIST Webbook
rinpol	3385.00		NIST Webbook
tb	1110.00	K	Joback Method
tc	1374.69	K	Joback Method
tf	743.56	K	Joback Method
vc	1.188	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	852.02	J/mol×K	1110.00	Joback Method
cpg	857.52	J/mol×K	1154.11	Joback Method
cpg	861.58	J/mol×K	1198.23	Joback Method
cpg	864.26	J/mol×K	1242.34	Joback Method
cpg	865.62	J/mol×K	1286.46	Joback Method
cpg	865.71	J/mol×K	1330.57	Joback Method
cpg	864.59	J/mol×K	1374.69	Joback Method
dvisc	0.0001280	Pa×s	743.56	Joback Method

dvisc	0.0000882	Pa×s	804.63	Joback Method
dvisc	0.0000640	Pa×s	865.71	Joback Method
dvisc	0.0000485	Pa×s	926.78	Joback Method
dvisc	0.0000380	Pa×s	987.85	Joback Method
dvisc	0.0000307	Pa×s	1048.93	Joback Method
dvisc	0.0000253	Pa×s	1110.00	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U382570&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
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

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