Phthalic acid, 2,4-dichlorobenzyl isobutyl ester

Inchi: InChI=1S/C19H18Cl2O4/c1-12(2)10-24-18(22)15-5-3-4-6-16(15)19(23)25-11-13-7-8-14(2

InchiKey: JMLNRSVUVOCUHU-UHFFFAOYSA-N

Formula: C19H18Cl2O4

SMILES: CC(C)COC(=O)c1ccccc1C(=O)OCc1ccc(Cl)cc1Cl

Mol. weight [g/mol]: 381.25

Physical Properties

Property code	Value	Unit	Source
gf	-189.11	kJ/mol	Joback Method
hf	-523.20	kJ/mol	Joback Method
hfus	42.33	kJ/mol	Joback Method
hvap	91.12	kJ/mol	Joback Method
log10ws	-6.45		Crippen Method
logp	5.163		Crippen Method
mcvol	270.410	ml/mol	McGowan Method
pc	1737.56	kPa	Joback Method
rinpol	2566.00		NIST Webbook
rinpol	2566.00		NIST Webbook
tb	929.42	K	Joback Method
tc	1166.09	K	Joback Method
tf	583.45	K	Joback Method
vc	1.024	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	766.38	J/mol×K	929.42	Joback Method
cpg	809.61	J/mol×K	1126.65	Joback Method
cpg	803.46	J/mol×K	1087.20	Joback Method
cpg	796.10	J/mol×K	1047.76	Joback Method
cpg	787.48	J/mol×K	1008.31	Joback Method
cpg	777.59	J/mol×K	968.87	Joback Method
cpg	814.58	J/mol×K	1166.09	Joback Method
dvisc	0.0000457	Pa×s	929.42	Joback Method

dvisc	0.0000570	Pa×s	871.76	Joback Method
dvisc	0.0000736	Pa×s	814.10	Joback Method
dvisc	0.0000986	Pa×s	756.44	Joback Method
dvisc	0.0001387	Pa×s	698.77	Joback Method
dvisc	0.0002076	Pa×s	641.11	Joback Method
dvisc	0.0003363	Pa×s	583.45	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U382559&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