Isophthalic acid, isobutyl phenyl ester

Inchi: InChI=1S/C18H18O4/c1-13(2)12-21-17(19)14-7-6-8-15(11-14)18(20)22-16-9-4-3-5-10-16
InchiKey: UAVWUYDEXWAJFS-UHFFFAOYSA-N
Formula: C18H18O4
SMILES: CC(C)COC(=O)c1cccc(C(=O)Oc2ccccc2)c1
Mol. weight [g/mol]: 298.33

Physical Properties

Property code	Value	Unit	Source
gf	-154.41	kJ/mol	Joback Method
hf	-448.14	kJ/mol	Joback Method
hfus	32.12	kJ/mol	Joback Method
hvap	78.80	kJ/mol	Joback Method
log10ws	-4.82		Crippen Method
logp	3.719		Crippen Method
mcvol	231.840	ml/mol	McGowan Method
pc	2068.00	kPa	Joback Method
rinpol	2416.00		NIST Webbook
rinpol	2416.00		NIST Webbook
tb	821.72	K	Joback Method
tc	1053.93	K	Joback Method
tf	487.30	K	Joback Method
vc	0.870	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	668.77	J/mol×K	821.72	Joback Method
cpg	726.92	J/mol×K	1015.23	Joback Method
cpg	717.75	J/mol×K	976.53	Joback Method
cpg	707.38	J/mol×K	937.82	Joback Method
cpg	695.79	J/mol×K	899.12	Joback Method
cpg	682.93	J/mol×K	860.42	Joback Method
cpg	734.93	J/mol×K	1053.93	Joback Method
dvisc	0.0000673	Pa×s	821.72	Joback Method

dvisc	0.0000862	Pa×s	765.98	Joback Method
dvisc	0.0001148	Pa×s	710.25	Joback Method
dvisc	0.0001605	Pa×s	654.51	Joback Method
dvisc	0.0002389	Pa×s	598.77	Joback Method
dvisc	0.0003858	Pa×s	543.04	Joback Method
dvisc	0.0006951	Pa×s	487.30	Joback Method

Sources

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=U344356&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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

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