Phthalic acid, 3,3-dimethylbut-2-yl isobutyl ester

Inchi: InChI=1S/C18H26O4/c1-12(2)11-21-16(19)14-9-7-8-10-15(14)17(20)22-13(3)18(4,5)6/h7
InchiKey: FYVGFDNOHPOTNO-UHFFFAOYSA-N
Formula: C18H26O4
SMILES: CC(C)COC(=O)c1ccccc1C(=O)OC(C)C(C)(C)C
Mol. weight [g/mol]: 306.40

Physical Properties

Property code	Value	Unit	Source
gf	-266.42	kJ/mol	Joback Method
hf	-698.70	kJ/mol	Joback Method
hfus	27.14	kJ/mol	Joback Method
hvap	74.84	kJ/mol	Joback Method
log10ws	-4.93		Crippen Method
logp	4.091		Crippen Method
mcvol	255.600	ml/mol	McGowan Method
pc	1596.17	kPa	Joback Method
rinpol	1981.00		NIST Webbook
tb	791.37	K	Joback Method
tc	1003.75	K	Joback Method
tf	448.30	K	Joback Method
vc	0.961	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	763.90	J/mol×K	791.37	Joback Method
cpg	834.26	J/mol×K	968.35	Joback Method
cpg	822.41	J/mol×K	932.96	Joback Method
cpg	809.48	J/mol×K	897.56	Joback Method
cpg	795.45	J/mol×K	862.16	Joback Method
cpg	780.27	J/mol×K	826.77	Joback Method
cpg	845.08	J/mol×K	1003.75	Joback Method
dvisc	0.0000490	Pa×s	791.37	Joback Method
dvisc	0.0000661	Pa×s	734.19	Joback Method

dvisc	0.0000938	Pa×s	677.01	Joback Method
dvisc	0.0001419	Pa×s	619.84	Joback Method
dvisc	0.0002336	Pa×s	562.66	Joback Method
dvisc	0.0004305	Pa×s	505.48	Joback Method
dvisc	0.0009271	Pa×s	448.30	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=U357001&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