Isophthalic acid, di(3,3-dimethylbut-2-yl) ester

Inchi: InChI=1S/C20H30O4/c1-13(19(3,4)5)23-17(21)15-10-9-11-16(12-15)18(22)24-14(2)20(6
InchiKey: NCIPBKKHYNJWNP-UHFFFAOYSA-N
Formula: C20H30O4
SMILES: CC(OC(=O)c1cccc(C(=O)OC(C)C(C)(C)C)c1)C(C)(C)C
Mol. weight [g/mol]: 334.45

Physical Properties

Property code	Value	Unit	Source
gf	-246.74	kJ/mol	Joback Method
hf	-748.73	kJ/mol	Joback Method
hfus	24.91	kJ/mol	Joback Method
hvap	78.00	kJ/mol	Joback Method
log10ws	-5.88		Crippen Method
logp	4.869		Crippen Method
mcvol	283.780	ml/mol	McGowan Method
pc	1396.46	kPa	Joback Method
rinpol	2138.00		NIST Webbook
tb	833.90	K	Joback Method
tc	1050.85	K	Joback Method
tf	473.26	K	Joback Method
vc	1.062	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	880.88	J/mol×K	833.90	Joback Method
cpg	953.48	J/mol×K	1014.69	Joback Method
cpg	941.23	J/mol×K	978.53	Joback Method
cpg	927.91	J/mol×K	942.37	Joback Method
cpg	913.46	J/mol×K	906.22	Joback Method
cpg	897.80	J/mol×K	870.06	Joback Method
cpg	964.74	J/mol×K	1050.85	Joback Method
dvisc	0.0000290	Pa×s	833.90	Joback Method
dvisc	0.0000400	Pa×s	773.79	Joback Method

dvisc	0.0000584	Pa×s	713.69	Joback Method
dvisc	0.0000913	Pa×s	653.58	Joback Method
dvisc	0.0001562	Pa×s	593.47	Joback Method
dvisc	0.0003019	Pa×s	533.37	Joback Method
dvisc	0.0006897	Pa×s	473.26	Joback Method

Sources

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

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=U356562&Units=SI

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