Isophthalic acid, 3,4-dimethylphenyl isobutyl ester

Inchi: InChI=1S/C20H22O4/c1-13(2)12-23-19(21)16-6-5-7-17(11-16)20(22)24-18-9-8-14(3)15(4

InchiKey: ZFOXOZRSIGJWTN-UHFFFAOYSA-N

Formula: C20H22O4

SMILES: Cc1ccc(OC(=O)c2cccc(C(=O)OCC(C)C)c2)cc1C

Mol. weight [g/mol]: 326.39

Physical Properties

Property code	Value	Unit	Source
gf	-156.83	kJ/mol	Joback Method
hf	-512.36	kJ/mol	Joback Method
hfus	36.52	kJ/mol	Joback Method
hvap	84.58	kJ/mol	Joback Method
log10ws	-5.77		Crippen Method
logp	4.335		Crippen Method
mcvol	260.020	ml/mol	McGowan Method
pc	1706.12	kPa	Joback Method
rinpol	2630.00		NIST Webbook
rinpol	2630.00		NIST Webbook
tb	877.44	K	Joback Method
tc	1105.63	K	Joback Method
tf	534.88	K	Joback Method
vc	0.982	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	779.75	J/mol×K	877.44	Joback Method
cpg	837.29	J/mol×K	1067.60	Joback Method
cpg	828.36	J/mol×K	1029.57	Joback Method
cpg	818.17	J/mol×K	991.53	Joback Method
cpg	806.69	J/mol×K	953.50	Joback Method
cpg	793.89	J/mol×K	915.47	Joback Method
cpg	844.97	J/mol×K	1105.63	Joback Method
dvisc	0.0000530	Pa×s	877.44	Joback Method

dvisc	0.0000667	Pa×s	820.35	Joback Method
dvisc	0.0000867	Pa×s	763.25	Joback Method
dvisc	0.0001176	Pa×s	706.16	Joback Method
dvisc	0.0001684	Pa×s	649.07	Joback Method
dvisc	0.0002584	Pa×s	591.97	Joback Method
dvisc	0.0004344	Pa×s	534.88	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U344440&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

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