Terephthalic acid, isobutyl 3-methoxyphenyl ester

Inchi: InChI=1S/C19H20O5/c1-13(2)12-23-18(20)14-7-9-15(10-8-14)19(21)24-17-6-4-5-16(11-1

InchiKey: ICEFDRJPOHXXOD-UHFFFAOYSA-N

Formula: C19H20O5

SMILES: COc1cccc(OC(=O)c2ccc(C(=O)OCC(C)C)cc2)c1

Mol. weight [g/mol]: 328.36

Physical Properties

Property code	Value	Unit	Source
gf	-260.62	kJ/mol	Joback Method
hf	-612.47	kJ/mol	Joback Method
hfus	35.51	kJ/mol	Joback Method
hvap	84.10	kJ/mol	Joback Method
log10ws	-4.93		Crippen Method
logp	3.727		Crippen Method
mcvol	251.800	ml/mol	McGowan Method
pc	1846.75	kPa	Joback Method
tb	872.00	K	Joback Method
tc	1100.23	K	Joback Method
tf	533.32	K	Joback Method
vc	0.944	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	750.72	J/mol×K	872.00	Joback Method
cpg	764.18	J/mol×K	910.04	Joback Method
cpg	776.25	J/mol×K	948.08	Joback Method
cpg	786.94	J/mol×K	986.11	Joback Method
cpg	796.26	J/mol×K	1024.15	Joback Method
cpg	804.23	J/mol×K	1062.19	Joback Method
cpg	810.84	J/mol×K	1100.23	Joback Method
dvisc	0.0003889	Pa×s	533.32	Joback Method
dvisc	0.0002286	Pa×s	589.77	Joback Method
dvisc	0.0001475	Pa×s	646.21	Joback Method

dvisc	0.0001021	Pa×s	702.66	Joback Method
dvisc	0.0000746	Pa×s	759.11	Joback Method
dvisc	0.0000570	Pa×s	815.55	Joback Method
dvisc	0.0000450	Pa×s	872.00	Joback Method

Sources

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=U415819&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume