1,4-Benzenedicarboxylic acid, bis(2-methylpropyl) ester

Other names: Terephthalic acid, diisobutyl ester
Diisobutyl terephthalate
Inchi: InChI=1S/C16H22O4/c1-11(2)9-19-15(17)13-5-7-14(8-6-13)16(18)20-10-12(3)4/h5-8,11-
InchiKey: LQKWPGAPADIOSS-UHFFFAOYSA-N
Formula: C16H22O4
SMILES: CC(C)COC(=O)c1ccc(C(=O)OCC(C)C)cc1
Mol. weight [g/mol]: 278.34
CAS: 18699-48-4

Physical Properties

Property code	Value	Unit	Source
gf	-286.10	kJ/mol	Joback Method
hf	-648.67	kJ/mol	Joback Method
hfus	29.38	kJ/mol	Joback Method
hvap	71.68	kJ/mol	Joback Method
log10ws	-3.98		Crippen Method
logp	3.312		Crippen Method
mcvol	227.420	ml/mol	McGowan Method
pc	1841.99	kPa	Joback Method
rinpol	1972.00		NIST Webbook
rinpol	1972.00		NIST Webbook
rinpol	1972.00		NIST Webbook
rinpol	1972.00		NIST Webbook
tb	748.84	K	Joback Method
tc	956.66	K	Joback Method
tf	423.34	K	Joback Method
vc	0.860	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	649.54	J/mol×K	748.84	Joback Method
cpg	665.13	J/mol×K	783.48	Joback Method
cpg	679.68	J/mol×K	818.11	Joback Method

cpg	693.19	J/mol×K	852.75	Joback Method
cpg	705.67	J/mol×K	887.39	Joback Method
cpg	717.14	J/mol×K	922.02	Joback Method
cpg	727.62	J/mol×K	956.66	Joback Method
dvisc	0.0011585	Pa×s	423.34	Joback Method
dvisc	0.0005749	Pa×s	477.59	Joback Method
dvisc	0.0003291	Pa×s	531.84	Joback Method
dvisc	0.0002089	Pa×s	586.09	Joback Method
dvisc	0.0001432	Pa×s	640.34	Joback Method
dvisc	0.0001042	Pa×s	694.59	Joback Method
dvisc	0.0000793	Pa×s	748.84	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=C18699484&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
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume