METHYL 4-(METHOXYCARBONYL)BENZYL TEREPHTHALATE

Other names: Methyl [4-(methoxycarbonyl)phenyl]methyl 1,4-benzenedicarboxylate
[4-(methoxycarbonyl)phenyl]methyl methyl terephthalate
Inchi: InChI=1S/C18H16O6/c1-22-16(19)13-5-3-12(4-6-13)11-24-18(21)15-9-7-14(8-10-15)17(2
InchiKey: ITTJRGPCQAAFGL-UHFFFAOYSA-N
Formula: C18H16O6
SMILES: COC(=O)c1ccc(COC(=O)c2ccc(C(=O)OC)cc2)cc1
Mol. weight [g/mol]: 328.32

Physical Properties

Property code	Value	Unit	Source
af	0.8972		Cheméo Relay (1.0)
hf	-844.23	kJ/mol	Cheméo Relay (1.0)
hfus	38.04	kJ/mol	Joback Method
hvap	112.40	kJ/mol	Cheméo Relay (1.0)
ie	9.39	eV	Cheméo Relay (1.0)
log10ws	-4.29		Cheméo Relay (1.0)
logp	2.617		Crippen Method
mcvol	239.280	ml/mol	McGowan Method
pc	2111.94	kPa	Joback Method
tb	651.15	K	Cheméo Relay (1.0)
tc	915.41	K	Cheméo Relay (1.0)
tf	356.20	K	Cheméo Relay (1.0)
vc	0.889	m3/kmol	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	702.63	J/mol×K	903.43	Joback Method
cpg	747.90	J/mol×K	1136.61	Joback Method
cpg	743.79	J/mol×K	1097.75	Joback Method
cpg	738.31	J/mol×K	1058.89	Joback Method
cpg	731.46	J/mol×K	1020.02	Joback Method
cpg	723.23	J/mol×K	981.16	Joback Method
cpg	713.62	J/mol×K	942.29	Joback Method

dvisc	0.0001122	Pa×s	745.20	Joback Method
dvisc	0.0000545	Pa×s	903.43	Joback Method
dvisc	0.0000673	Pa×s	850.69	Joback Method
dvisc	0.0000854	Pa×s	797.95	Joback Method
dvisc	0.0003411	Pa×s	586.98	Joback Method
dvisc	0.0001536	Pa×s	692.46	Joback Method
dvisc	0.0002215	Pa×s	639.72	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Cheméo Relay (1.0):	
Cheméo Relay (1.0, beta):	
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C55334515&Units=SI
Joback Method:	https://en.wikipedia.org/wiki/Joback_method

Legend

af:	Acentric Factor
cpg:	Ideal gas heat capacity
dvisc:	Dynamic viscosity
hf:	Enthalpy of formation at standard conditions
hfus:	Enthalpy of fusion at standard conditions
hvap:	Enthalpy of vaporization at standard conditions
ie:	Ionization energy
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