1,4-Benzenedicarboxylic acid, [4-(methoxycarbonyl)phenyl]methyl methyl ester

Othernames: 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

CAS: 55334-51-5

Physical Properties

Property code	Value	Unit	Source
gf	-395.52	kJ/mol	Joback Method
hf	-699.13	kJ/mol	Joback Method
hfus	38.04	kJ/mol	Joback Method
hvap	89.01	kJ/mol	Joback Method
log10ws	-4.31		Crippen Method
logp	2.617		Crippen Method
mcvol	239.280	ml/mol	McGowan Method
pc	2111.94	kPa	Joback Method
tb	903.43	K	Joback Method
tc	1136.61	K	Joback Method
tf	586.98	K	Joback Method
vc	0.899	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	702.63	J/mol×K	903.43	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
cpg	747.90	J/mol×K	1136.61	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	0.0001122	Pa×s	745.20	Joback Method
dvisc	0.0001536	Pa×s	692.46	Joback Method
dvisc	0.0002215	Pa×s	639.72	Joback Method
dvisc	0.0003411	Pa×s	586.98	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=C55334515&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

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