Methyl 4-methylpentyl phthalate

Other names: 1,2-Benzenedicarboxylic acid, 4-methylpentyl methyl ester
Inchi: InChI=1S/C15H20O4/c1-11(2)7-6-10-19-15(17)13-9-5-4-8-12(13)14(16)18-3/h4-5,8-9,11
InchiKey: ZNWQXIZPCPQPTJ-UHFFFAOYSA-N
Formula: C15H20O4
SMILES: COC(=O)c1ccccc1C(=O)OCCCC(C)C
Mol. weight [g/mol]: 264.32

Physical Properties

Property code	Value	Unit	Source
gf	-292.08	kJ/mol	Joback Method
hf	-622.75	kJ/mol	Joback Method
hfus	30.31	kJ/mol	Joback Method
hvap	69.85	kJ/mol	Joback Method
log10ws	-3.81		Crippen Method
logp	3.066		Crippen Method
mcvol	213.330	ml/mol	McGowan Method
pc	1989.43	kPa	Joback Method
rinpol	1898.00		NIST Webbook
rinpol	1898.00		NIST Webbook
tb	726.40	K	Joback Method
tc	933.26	K	Joback Method
tf	427.07	K	Joback Method
vc	0.809	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	594.17	J/mol×K	726.40	Joback Method
cpg	659.69	J/mol×K	898.78	Joback Method
cpg	648.50	J/mol×K	864.30	Joback Method
cpg	636.36	J/mol×K	829.83	Joback Method
cpg	623.26	J/mol×K	795.35	Joback Method
cpg	609.21	J/mol×K	760.88	Joback Method
cpg	669.96	J/mol×K	933.26	Joback Method

dvisc	0.0000976	Pa×s	726.40	Joback Method
dvisc	0.0001255	Pa×s	676.51	Joback Method
dvisc	0.0001681	Pa×s	626.62	Joback Method
dvisc	0.0002367	Pa×s	576.74	Joback Method
dvisc	0.0003556	Pa×s	526.85	Joback Method
dvisc	0.0005817	Pa×s	476.96	Joback Method
dvisc	0.0010677	Pa×s	427.07	Joback Method

Sources

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
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U373826&Units=SI

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