Phthalic acid, methyl octyl ester

Other names: 1,2-Benzenedicarboxylic acid, octyl methyl ester
Octyl methyl phthalate
Inchi: InChI=1S/C17H24O4/c1-3-4-5-6-7-10-13-21-17(19)15-12-9-8-11-14(15)16(18)20-2/h8-9,
InchiKey: SJMMDRTYFFDPBJ-UHFFFAOYSA-N
Formula: C17H24O4
SMILES: CCCCCCCCOC(=O)c1ccccc1C(=O)OC
Mol. weight [g/mol]: 292.37

Physical Properties

Property code	Value	Unit	Source
af	0.8909		Cheméo Relay (1.0)
hf	-743.67	kJ/mol	Cheméo Relay (1.0)
hfus	39.01	kJ/mol	Joback Method
hvap	90.41	kJ/mol	Cheméo Relay (1.0)
ie	9.17	eV	Cheméo Relay (1.0)
log10ws	-5.08		Cheméo Relay (1.0)
logp	3.990		Crippen Method
mcvol	241.510	ml/mol	McGowan Method
pc	1676.91	kPa	Joback Method
tb	606.48	K	Cheméo Relay (1.0)
tc	811.91	K	Cheméo Relay (1.0)
tf	267.55	K	Cheméo Relay (1.0)
vc	0.908	m3/kmol	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	704.35	J/mol×K	772.60	Joback Method
cpg	719.77	J/mol×K	806.01	Joback Method
cpg	734.18	J/mol×K	839.41	Joback Method
cpg	747.59	J/mol×K	872.82	Joback Method
cpg	760.03	J/mol×K	906.23	Joback Method
cpg	771.51	J/mol×K	939.63	Joback Method
cpg	782.03	J/mol×K	973.04	Joback Method

dvisc	0.0007844	Pa×s	464.61	Joback Method
dvisc	0.0004467	Pa×s	515.94	Joback Method
dvisc	0.0002816	Pa×s	567.27	Joback Method
dvisc	0.0001917	Pa×s	618.61	Joback Method
dvisc	0.0001384	Pa×s	669.94	Joback Method
dvisc	0.0001047	Pa×s	721.27	Joback Method
dvisc	0.0000821	Pa×s	772.60	Joback Method

Sources

Joback Method:	https://en.wikipedia.org/wiki/Joback_method
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=C91485835&Units=SI

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