Methyl octyl phthalate

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
CAS: 91485-83-5

Physical Properties

Property code	Value	Unit	Source
gf	-272.80	kJ/mol	Joback Method
hf	-658.75	kJ/mol	Joback Method
hfus	39.01	kJ/mol	Joback Method
hvap	74.69	kJ/mol	Joback Method
log10ws	-4.89		Crippen Method
logp	3.990		Crippen Method
mcvol	241.510	ml/mol	McGowan Method
pc	1676.91	kPa	Joback Method
rinpol	2141.00		NIST Webbook
tb	772.60	K	Joback Method
tc	973.04	K	Joback Method
tf	464.61	K	Joback Method
vc	0.927	m3/kmol	Joback Method

Temperature Dependent Properties

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

cpg	782.03	J/mol×K	973.04	Joback Method
dvisc	0.0000821	Pa×s	772.60	Joback Method
dvisc	0.0001047	Pa×s	721.27	Joback Method
dvisc	0.0001384	Pa×s	669.94	Joback Method
dvisc	0.0001917	Pa×s	618.61	Joback Method
dvisc	0.0002816	Pa×s	567.27	Joback Method
dvisc	0.0004467	Pa×s	515.94	Joback Method
dvisc	0.0007844	Pa×s	464.61	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=C91485835&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

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