1-Methyl-2-methoxyethyl 2-phenoxybenzoate

Inchi: InChI=1S/C17H18O4/c1-13(12-19-2)20-17(18)15-10-6-7-11-16(15)21-14-8-4-3-5-9-14/h3
InchiKey: QHGPFODYBMARQS-UHFFFAOYSA-N
Formula: C17H18O4
SMILES: COCC(C)OC(=O)c1ccccc1Oc1ccccc1
Mol. weight [g/mol]: 286.32

Physical Properties

Property code	Value	Unit	Source
gf	-138.91	kJ/mol	Joback Method
hf	-447.14	kJ/mol	Joback Method
hfus	29.12	kJ/mol	Joback Method
hvap	72.24	kJ/mol	Joback Method
log10ws	-3.80		Crippen Method
logp	3.671		Crippen Method
mcvol	222.050	ml/mol	McGowan Method
pc	2098.42	kPa	Joback Method
rinpol	1976.00		NIST Webbook
rinpol	1976.00		NIST Webbook
tb	767.39	K	Joback Method
tc	995.25	K	Joback Method
tf	448.33	K	Joback Method
vc	0.826	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	626.09	J/mol×K	767.39	Joback Method
cpg	641.61	J/mol×K	805.37	Joback Method
cpg	655.84	J/mol×K	843.34	Joback Method
cpg	668.81	J/mol×K	881.32	Joback Method
cpg	680.53	J/mol×K	919.30	Joback Method
cpg	691.01	J/mol×K	957.27	Joback Method
cpg	700.27	J/mol×K	995.25	Joback Method
dvisc	0.0006511	Pa×s	448.33	Joback Method

dvisc	0.0003540	Pa×s	501.51	Joback Method
dvisc	0.0002163	Pa×s	554.68	Joback Method
dvisc	0.0001440	Pa×s	607.86	Joback Method
dvisc	0.0001024	Pa×s	661.04	Joback Method
dvisc	0.0000766	Pa×s	714.21	Joback Method
dvisc	0.0000597	Pa×s	767.39	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=R540024&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
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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