

2-Methoxyethyl methyl phthalate

Other names:	1,2-Benzenedicarboxylic acid, 2-methoxyethyl methyl ester
Inchi:	InChI=1S/C12H14O5/c1-15-7-8-17-12(14)10-6-4-3-5-9(10)11(13)16-2/h3-6H,7-8H2,1-2H1
InchiKey:	DRYXMSSOAFCHRL-UHFFFAOYSA-N
Formula:	C12H14O5
SMILES:	COCCOC(=O)c1cccc1C(=O)OC
Mol. weight [g/mol]:	238.24

Physical Properties

Property code	Value	Unit	Source
gf	-419.90	kJ/mol	Joback Method
hf	-687.77	kJ/mol	Joback Method
hfus	27.25	kJ/mol	Joback Method
hvap	65.97	kJ/mol	Joback Method
log10ws	-1.88		Crippen Method
logp	1.276		Crippen Method
mcvol	176.930	ml/mol	McGowan Method
pc	2553.34	kPa	Joback Method
rinpol	1755.00		NIST Webbook
tb	680.62	K	Joback Method
tc	890.28	K	Joback Method
tf	430.49	K	Joback Method
vc	0.665	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	461.71	J/mol×K	680.62	Joback Method
cpg	474.82	J/mol×K	715.56	Joback Method
cpg	487.13	J/mol×K	750.51	Joback Method
cpg	498.62	J/mol×K	785.45	Joback Method
cpg	509.27	J/mol×K	820.39	Joback Method
cpg	519.08	J/mol×K	855.34	Joback Method
cpg	528.02	J/mol×K	890.28	Joback Method
dvisc	0.0008188	Pa×s	430.49	Joback Method

dvisc	0.0005128	Pa×s	472.18	Joback Method
dvisc	0.0003465	Pa×s	513.87	Joback Method
dvisc	0.0002484	Pa×s	555.56	Joback Method
dvisc	0.0001865	Pa×s	597.24	Joback Method
dvisc	0.0001453	Pa×s	638.93	Joback Method
dvisc	0.0001168	Pa×s	680.62	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=U373894&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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