Phthalic acid, monoethyl ester

Other names:	1,2-Benzenecarboxylic acid, monoethyl ester
	Monoethyl phthalate
	2-(Ethoxycarbonyl)benzoic acid
Inchi:	InChI=1S/C10H10O4/c1-2-14-10(13)8-6-4-3-5-7(8)9(11)12/h3-6H,2H2,1H3,(H,11,12)
InchiKey:	YWWHKOHZGJFMIE-UHFFFAOYSA-N
Formula:	C10H10O4
SMILES:	CCOC(=O)c1ccccc1C(=O)O
Mol. weight [g/mol]:	194.18
CAS:	2306-33-4

Physical Properties

Property code	Value	Unit	Source
gf	-363.56	kJ/mol	Joback Method
hf	-534.28	kJ/mol	Joback Method
hfus	23.78	kJ/mol	Joback Method
hvap	73.37	kJ/mol	Joback Method
log10ws	-2.19		Crippen Method
logp	1.561		Crippen Method
mcvol	142.880	ml/mol	McGowan Method
pc	3624.61	kPa	Joback Method
rinpol	1651.00		NIST Webbook
rinpol	1651.00		NIST Webbook
tb	682.20	K	Joback Method
tc	888.42	K	Joback Method
tf	424.31	K	Joback Method
vc	0.536	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	361.74	J/mol×K	682.20	Joback Method
cpg	404.35	J/mol×K	854.05	Joback Method
cpg	397.06	J/mol×K	819.68	Joback Method
cpg	389.16	J/mol×K	785.31	Joback Method

cpg	380.65	J/mol×K	750.94	Joback Method
cpg	371.51	J/mol×K	716.57	Joback Method
cpg	411.06	J/mol×K	888.42	Joback Method
dvisc	0.0000584	Pa×s	682.20	Joback Method
dvisc	0.0000831	Pa×s	639.22	Joback Method
dvisc	0.0001242	Pa×s	596.24	Joback Method
dvisc	0.0001977	Pa×s	553.25	Joback Method
dvisc	0.0003404	Pa×s	510.27	Joback Method
dvisc	0.0006477	Pa×s	467.29	Joback Method
dvisc	0.0014037	Pa×s	424.31	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=C2306334&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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