4-METHOXYPHENYLACETIC ACID, ETHYL ESTER

Other names: Ethyl 4-methoxyphenylacetate
p-Methoxyphenylacetic acid ethyl ester
Benzeneacetic acid, 4-methoxy-, ethyl ester

Inchi: InChI=1S/C11H14O3/c1-3-14-11(12)8-9-4-6-10(13-2)7-5-9/h4-7H,3,8H2,1-2H3

InchiKey: DOCCDOCIYYDLGJ-UHFFFAOYSA-N

Formula: C11H14O3

SMILES: CCOC(=O)Cc1ccc(OC)cc1

Mol. weight [g/mol]: 194.23

Physical Properties

Property code	Value	Unit	Source
af	0.5975		Cheméo Relay (1.0)
gf	-194.40	kJ/mol	Joback Method
hf	-474.47	kJ/mol	Cheméo Relay (1.0)
hfus	21.87	kJ/mol	Joback Method
hvap	72.32	kJ/mol	Cheméo Relay (1.0)
ie	7.85	eV	Cheméo Relay (1.0)
log10ws	-2.56		Cheméo Relay (1.0)
logp	1.801		Crippen Method
mcvol	155.400	ml/mol	McGowan Method
pc	2687.42	kPa	Joback Method
tb	551.74	K	Cheméo Relay (1.0)
tc	741.13	K	Cheméo Relay (1.0)
tf	282.13	K	Cheméo Relay (1.0)
vc	0.574	m3/kmol	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	370.80	J/mol×K	581.45	Joback Method
cpg	443.58	J/mol×K	789.55	Joback Method
cpg	433.22	J/mol×K	754.87	Joback Method
cpg	422.16	J/mol×K	720.18	Joback Method
cpg	410.38	J/mol×K	685.50	Joback Method

cpg	397.90	J/mol×K	650.82	Joback Method
cpg	384.70	J/mol×K	616.13	Joback Method
dvisc	0.0003501	Pa×s	464.25	Joback Method
dvisc	0.0001589	Pa×s	581.45	Joback Method
dvisc	0.0001991	Pa×s	542.38	Joback Method
dvisc	0.0002583	Pa×s	503.32	Joback Method
dvisc	0.0013141	Pa×s	347.06	Joback Method
dvisc	0.0005017	Pa×s	425.19	Joback Method
dvisc	0.0007734	Pa×s	386.12	Joback Method

Sources

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=C14062181&Units=SI
Joback Method: https://en.wikipedia.org/wiki/Joback_method
McGowan Method: http://link.springer.com/article/10.1007/BF02311772

Legend

af: Acentric Factor
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
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