ANISYL PHENYLACETATE

Other names:	Acetic acid, phenyl-, p-methoxybenzyl ester
	p-Anisyl phenylacetate
	p-Methoxybenzyl phenylacetate
	Phenylacetic acid, p-methoxybenzyl ester
	4-methoxybenzyl phenylacetate
Inchi:	InChI=1S/C16H16O3/c1-18-15-9-7-14(8-10-15)12-19-16(17)11-13-5-3-2-4-6-13/h2-10H,1
InchiKey:	VCYWCSZLXMMLLE-UHFFFAOYSA-N
Formula:	C16H16O3
SMILES:	COc1ccc(COC(=O)Cc2ccccc2)cc1
Mol. weight [g/mol]:	256.30

Physical Properties

Property code	Value	Unit	Source
hf	-310.73	kJ/mol	Cheméo Relay (1.0)
hfus	28.86	kJ/mol	Joback Method
hvap	92.15	kJ/mol	Cheméo Relay (1.0)
ie	7.96	eV	Cheméo Relay (1.0)
log10ws	-3.89		Cheméo Relay (1.0)
logp	2.981		Crippen Method
mcvol	202.090	ml/mol	McGowan Method
pc	2315.84	kPa	Joback Method
tb	622.85	K	Cheméo Relay (1.0)
tf	312.19	K	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	544.43	J/mol×K	722.53	Joback Method
cpg	559.93	J/mol×K	760.96	Joback Method
cpg	574.23	J/mol×K	799.38	Joback Method
cpg	587.37	J/mol×K	837.81	Joback Method
cpg	599.38	J/mol×K	876.23	Joback Method
cpg	610.29	J/mol×K	914.66	Joback Method
cpg	620.12	J/mol×K	953.08	Joback Method

dvisc	0.0008483	Pa×s	429.83	Joback Method
dvisc	0.0004890	Pa×s	478.61	Joback Method
dvisc	0.0003121	Pa×s	527.40	Joback Method
dvisc	0.0002150	Pa×s	576.18	Joback Method
dvisc	0.0001569	Pa×s	624.96	Joback Method
dvisc	0.0001199	Pa×s	673.75	Joback Method
dvisc	0.0000950	Pa×s	722.53	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
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=C102170&Units=SI
Joback Method:	https://en.wikipedia.org/wiki/Joback_method

Legend

cpg:	Ideal gas heat capacity
dvisc:	Dynamic viscosity
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
tf:	Normal melting (fusion) point