Anisyl acetate

Other names: Benzenemethanol, 4-methoxy-, acetate
p-anisyl acetate
Inchi: InChI=1S/C10H12O3/c1-8(11)13-7-9-3-5-10(12-2)6-4-9/h3-6H,7H2,1-2H3
InchiKey: HFNGYHHRRMSKEU-UHFFFAOYSA-N
Formula: C10H12O3
SMILES: COc1ccc(COC(C)=O)cc1
Mol. weight [g/mol]: 180.20
CAS: 1331-83-5

Physical Properties

Property code	Value	Unit	Source
gf	-202.82	kJ/mol	Joback Method
hf	-401.69	kJ/mol	Joback Method
hfus	19.28	kJ/mol	Joback Method
hvap	52.36	kJ/mol	Joback Method
log10ws	-2.17		Crippen Method
logp	1.758		Crippen Method
mcvol	141.310	ml/mol	McGowan Method
pc	2976.29	kPa	Joback Method
rinpol	1387.00		NIST Webbook
rinpol	1426.00		NIST Webbook
rinpol	1380.00		NIST Webbook
rinpol	1419.00		NIST Webbook
rinpol	1376.00		NIST Webbook
rinpol	1382.50		NIST Webbook
rinpol	1413.00		NIST Webbook
rinpol	1390.00		NIST Webbook
rinpol	1426.00		NIST Webbook
rinpol	1376.00		NIST Webbook
rinpol	1426.00		NIST Webbook
rinpol	1387.00		NIST Webbook
rinpol	1382.00		NIST Webbook
rinpol	1376.00		NIST Webbook
ripol	2199.00		NIST Webbook
tb	558.57	K	Joback Method
tc	770.06	K	Joback Method
tf	335.79	K	Joback Method

vc	0.529	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	323.98	J/mol×K	558.57	Joback Method
cpg	337.02	J/mol×K	593.82	Joback Method
cpg	349.42	J/mol×K	629.07	Joback Method
cpg	361.16	J/mol×K	664.31	Joback Method
cpg	372.24	J/mol×K	699.56	Joback Method
cpg	382.66	J/mol×K	734.81	Joback Method
cpg	392.43	J/mol×K	770.06	Joback Method
dvisc	0.0013400	Pa×s	335.79	Joback Method
dvisc	0.0008036	Pa×s	372.92	Joback Method
dvisc	0.0005287	Pa×s	410.05	Joback Method
dvisc	0.0003728	Pa×s	447.18	Joback Method
dvisc	0.0002774	Pa×s	484.31	Joback Method
dvisc	0.0002153	Pa×s	521.44	Joback Method
dvisc	0.0001728	Pa×s	558.57	Joback Method

Sources

McGowan Method: http://link.springer.com/article/10.1007/BF02311772
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C1331835&Units=SI
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

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
ripol:	Polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume