Amyl anisate

Other names:	Anisic acid, pentyl ester
	Benzoic acid, 4-methoxy-, pentyl ester
	p-Methoxybenzoic acid, pentyl ester
	n-Amyl anisoate
	Pentyl 4-methoxybenzoate
Inchi:	InChI=1S/C13H18O3/c1-3-4-5-10-16-13(14)11-6-8-12(15-2)9-7-11/h6-9H,3-5,10H2,1-2H
InchiKey:	DNJKWCMASVISFH-UHFFFAOYSA-N
Formula:	C13H18O3
SMILES:	CCCCCOC(=O)c1ccc(OC)cc1
Mol. weight [g/mol]:	222.28
CAS:	6938-46-1

Physical Properties

Property code	Value	Unit	Source
gf	-177.56	kJ/mol	Joback Method
hf	-463.61	kJ/mol	Joback Method
hfus	27.05	kJ/mol	Joback Method
hvap	59.04	kJ/mol	Joback Method
log10ws	-3.51		Crippen Method
logp	3.042		Crippen Method
mcvol	183.580	ml/mol	McGowan Method
pc	2222.89	kPa	Joback Method
rinpol	1763.70		NIST Webbook
rinpol	1781.00		NIST Webbook
rinpol	1727.00		NIST Webbook
rinpol	1732.00		NIST Webbook
ripol	2405.00		NIST Webbook
ripol	2393.00		NIST Webbook
tb	627.21	K	Joback Method
tc	829.16	K	Joback Method
tf	369.60	K	Joback Method
vc	0.698	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	469.42	J/mol×K	627.21	Joback Method
cpg	537.75	J/mol×K	795.50	Joback Method
cpg	525.67	J/mol×K	761.85	Joback Method
cpg	512.81	J/mol×K	728.19	Joback Method
cpg	499.15	J/mol×K	694.53	Joback Method
cpg	484.69	J/mol×K	660.87	Joback Method
cpg	549.04	J/mol×K	829.16	Joback Method
dvisc	0.0001313	Pa×s	627.21	Joback Method
dvisc	0.0001661	Pa×s	584.28	Joback Method
dvisc	0.0002181	Pa×s	541.34	Joback Method
dvisc	0.0003002	Pa×s	498.41	Joback Method
dvisc	0.0004388	Pa×s	455.47	Joback Method
dvisc	0.0006941	Pa×s	412.54	Joback Method
dvisc	0.0012215	Pa×s	369.60	Joback Method

Sources

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=C6938461&Units=SI
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

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