o-Methoxybenzoic acid, pentyl ester

Other names: o-Methoxybenzoic acid, pentyl ester
Pentyl 2-methoxybenzoate
pentyl o-anisate
Inchi: InChI=1S/C13H18O3/c1-3-4-7-10-16-13(14)11-8-5-6-9-12(11)15-2/h5-6,8-9H,3-4,7,10H2
InchiKey: TYLMQMJLOUNOGK-UHFFFAOYSA-N
Formula: C13H18O3
SMILES: CCCCCOC(=O)c1ccccc1OC
Mol. weight [g/mol]: 222.28

Physical Properties

Property code	Value	Unit	Source
af	0.7098		Cheméo Relay (1.0)
hf	-502.87	kJ/mol	Cheméo Relay (1.0)
hfus	27.05	kJ/mol	Joback Method
hvap	74.05	kJ/mol	Cheméo Relay (1.0)
log10ws	-3.91		Cheméo Relay (1.0)
logp	3.042		Crippen Method
mcvol	183.580	ml/mol	McGowan Method
pc	2222.89	kPa	Joback Method
rinpol	1710.00		NIST Webbook
rinpol	1700.60		NIST Webbook
rinpol	1710.00		NIST Webbook
tb	572.04	K	Cheméo Relay (1.0)
tc	760.91	K	Cheméo Relay (1.0)
tf	260.69	K	Cheméo Relay (1.0)
vc	0.683	m3/kmol	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	469.42	J/mol×K	627.21	Joback Method
cpg	484.69	J/mol×K	660.87	Joback Method
cpg	499.15	J/mol×K	694.53	Joback Method
cpg	512.81	J/mol×K	728.19	Joback Method

cpg	525.67	J/mol×K	761.85	Joback Method
cpg	537.75	J/mol×K	795.50	Joback Method
cpg	549.04	J/mol×K	829.16	Joback Method
dvisc	0.0012215	Pa×s	369.60	Joback Method
dvisc	0.0006941	Pa×s	412.54	Joback Method
dvisc	0.0004388	Pa×s	455.47	Joback Method
dvisc	0.0003002	Pa×s	498.41	Joback Method
dvisc	0.0002181	Pa×s	541.34	Joback Method
dvisc	0.0001661	Pa×s	584.28	Joback Method
dvisc	0.0001313	Pa×s	627.21	Joback Method

Sources

Joback Method:	https://en.wikipedia.org/wiki/Joback_method
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=C22708141&Units=SI

Legend

af:	Acentric Factor
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
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