Benzoic acid, 2-methoxy-, 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
CAS: 22708-14-1

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	1710.00		NIST Webbook
rinpol	1710.00		NIST Webbook
rinpol	1700.60		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	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

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=C22708141&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
tb: Normal Boiling Point Temperature
tc: Critical Temperature
tf: Normal melting (fusion) point
vc: Critical Volume