

Benzoic acid, 3-pentyloxy-, methyl ester

Inchi:	InChI=1S/C13H18O3/c1-3-4-5-9-16-12-8-6-7-11(10-12)13(14)15-2/h6-8,10H,3-5,9H2,1-2
InchiKey:	VLGBMUPRDSTBKL-UHFFFAOYSA-N
Formula:	C13H18O3
SMILES:	CCCCCOc1cccc(C(=O)OC)c1
Mol. weight [g/mol]:	222.28

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
mvol	183.580	ml/mol	McGowan Method
pc	2222.89	kPa	Joback Method
rinpol	1738.00		NIST Webbook
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tb	627.21	K	Joback Method
tc	829.16	K	Joback Method
tf	369.60	K	Joback Method
vc	0.698	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	469.42	J/molxK	627.21	Joback Method
cpg	484.69	J/molxK	660.87	Joback Method
cpg	499.15	J/molxK	694.53	Joback Method
cpg	512.81	J/molxK	728.19	Joback Method
cpg	525.67	J/molxK	761.85	Joback Method
cpg	537.75	J/molxK	795.50	Joback Method
cpg	549.04	J/molxK	829.16	Joback Method
dvisc	0.0012215	Paxs	369.60	Joback Method

dvisc	0.0006941	Paxs	412.54	Joback Method
dvisc	0.0004388	Paxs	455.47	Joback Method
dvisc	0.0003002	Paxs	498.41	Joback Method
dvisc	0.0002181	Paxs	541.34	Joback Method
dvisc	0.0001661	Paxs	584.28	Joback Method
dvisc	0.0001313	Paxs	627.21	Joback Method

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
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=U374359&Units=SI

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

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