Formic acid, 5-methoxy-3-phenylpentyl ester

Inchi: InChI=1S/C13H18O3/c1-15-9-7-13(8-10-16-11-14)12-5-3-2-4-6-12/h2-6,11,13H,7-10H2,1
InchiKey: KBGIXBCGHBVUDU-UHFFFAOYSA-N
Formula: C13H18O3
SMILES: COCCC(CCOC=O)c1ccccc1
Mol. weight [g/mol]: 222.28

Physical Properties

Property code	Value	Unit	Source
gf	-140.97	kJ/mol	Joback Method
hf	-430.42	kJ/mol	Joback Method
hfus	24.61	kJ/mol	Joback Method
hvap	57.96	kJ/mol	Joback Method
log10ws	-2.28		Crippen Method
logp	2.370		Crippen Method
mcvol	183.580	ml/mol	McGowan Method
pc	2295.91	kPa	Joback Method
rinpol	1616.00		NIST Webbook
rinpol	1616.00		NIST Webbook
tb	616.58	K	Joback Method
tc	817.20	K	Joback Method
tf	334.15	K	Joback Method
vc	0.703	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	470.53	J/mol×K	616.58	Joback Method
cpg	539.64	J/mol×K	783.76	Joback Method
cpg	527.46	J/mol×K	750.32	Joback Method
cpg	514.47	J/mol×K	716.89	Joback Method
cpg	500.66	J/mol×K	683.45	Joback Method
cpg	486.02	J/mol×K	650.02	Joback Method
cpg	551.03	J/mol×K	817.20	Joback Method
dvisc	0.0001369	Pa×s	616.58	Joback Method

dvisc	0.0001800	Pa×s	569.51	Joback Method
dvisc	0.0002487	Pa×s	522.44	Joback Method
dvisc	0.0003662	Pa×s	475.37	Joback Method
dvisc	0.0005873	Pa×s	428.29	Joback Method
dvisc	0.0010583	Pa×s	381.22	Joback Method
dvisc	0.0022512	Pa×s	334.15	Joback Method

Sources

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=U368757&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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