Benzoic acid,4-propyloxy, methyl ester

Other names:	Methyl 4-propoxybenzoate
	Benzoic acid, 4-propoxy-, methyl ester
	methyl 4-n-propoxybenzoate
Inchi:	InChI=1S/C11H14O3/c1-3-8-14-10-6-4-9(5-7-10)11(12)13-2/h4-7H,3,8H2,1-2H3
InchiKey:	OXOTVVQIIASDNF-UHFFFAOYSA-N
Formula:	C11H14O3
SMILES:	CCCOc1ccc(C(=O)OC)cc1
Mol. weight [g/mol]:	194.23
CAS:	115478-59-6

Physical Properties

Property code	Value	Unit	Source
gf	-194.40	kJ/mol	Joback Method
hf	-422.33	kJ/mol	Joback Method
hfus	21.87	kJ/mol	Joback Method
hvap	54.58	kJ/mol	Joback Method
log10ws	-2.67		Crippen Method
logp	2.262		Crippen Method
mcvol	155.400	ml/mol	McGowan Method
pc	2687.42	kPa	Joback Method
rinpol	1567.00		NIST Webbook
tb	581.45	K	Joback Method
tc	789.55	K	Joback Method
tf	347.06	K	Joback Method
vc	0.586	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	370.80	J/mol×K	581.45	Joback Method
cpg	433.22	J/mol×K	754.87	Joback Method
cpg	422.16	J/mol×K	720.18	Joback Method
cpg	410.38	J/mol×K	685.50	Joback Method
cpg	397.90	J/mol×K	650.82	Joback Method

cpg	384.70	J/mol×K	616.13	Joback Method
cpg	443.58	J/mol×K	789.55	Joback Method
dvisc	0.0001589	Pa×s	581.45	Joback Method
dvisc	0.0001991	Pa×s	542.38	Joback Method
dvisc	0.0002583	Pa×s	503.32	Joback Method
dvisc	0.0003501	Pa×s	464.25	Joback Method
dvisc	0.0005017	Pa×s	425.19	Joback Method
dvisc	0.0007734	Pa×s	386.12	Joback Method
dvisc	0.0013141	Pa×s	347.06	Joback Method

Sources

Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l
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=C115478596&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