

Benzoic acid, 3-propyloxy-, methyl ester

Inchi:	InChI=1S/C11H14O3/c1-3-7-14-10-6-4-5-9(8-10)11(12)13-2/h4-6,8H,3,7H2,1-2H3
InchiKey:	JAVSSVQOQMMSTI-UHFFFAOYSA-N
Formula:	C11H14O3
SMILES:	CCCOc1cccc(C(=O)OC)c1
Mol. weight [g/mol]:	194.23

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	1533.00		NIST Webbook
rinpol	1533.00		NIST Webbook
tb	581.45	K	Joback Method
tc	789.55	K	Joback Method
tf	347.06	K	Joback Method
vc	0.586	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	370.80	J/molxK	581.45	Joback Method
cpg	384.70	J/molxK	616.13	Joback Method
cpg	397.90	J/molxK	650.82	Joback Method
cpg	410.38	J/molxK	685.50	Joback Method
cpg	422.16	J/molxK	720.18	Joback Method
cpg	433.22	J/molxK	754.87	Joback Method
cpg	443.58	J/molxK	789.55	Joback Method
dvisc	0.0013141	Paxs	347.06	Joback Method

dvisc	0.0007734	Paxs	386.12	Joback Method
dvisc	0.0005017	Paxs	425.19	Joback Method
dvisc	0.0003501	Paxs	464.25	Joback Method
dvisc	0.0002583	Paxs	503.32	Joback Method
dvisc	0.0001991	Paxs	542.38	Joback Method
dvisc	0.0001589	Paxs	581.45	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=U374499&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071

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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