Benzoic acid, 2-ethoxy-, methyl ester

Other names:	Benzoic acid, o-ethoxy-, methyl ester
	Methyl o-ethoxybenzoate
	R 172 (The insectifuge)
	Methyl 2-ethoxybenzoate
	R 172
Inchi:	InChI=1S/C10H12O3/c1-3-13-9-7-5-4-6-8(9)10(11)12-2/h4-7H,3H2,1-2H3
InchiKey:	QAYQKAPOTVSWLS-UHFFFAOYSA-N
Formula:	C10H12O3
SMILES:	CCOc1ccccc1C(=O)OC
Mol. weight [g/mol]:	180.20
CAS:	3686-55-3

Physical Properties

Property code	Value	Unit	Source
gf	-202.82	kJ/mol	Joback Method
hf	-401.69	kJ/mol	Joback Method
hfus	19.28	kJ/mol	Joback Method
hvap	52.36	kJ/mol	Joback Method
log10ws	-2.25		Crippen Method
logp	1.872		Crippen Method
mcvol	141.310	ml/mol	McGowan Method
pc	2976.29	kPa	Joback Method
rinpol	1347.00		NIST Webbook
rinpol	1394.00		NIST Webbook
rinpol	1351.00		NIST Webbook
tb	558.57	K	Joback Method
tc	770.06	K	Joback Method
tf	335.79	K	Joback Method
vc	0.529	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	323.98	J/mol×K	558.57	Joback Method

cpg	382.66	J/mol×K	734.81	Joback Method
cpg	372.24	J/mol×K	699.56	Joback Method
cpg	361.16	J/mol×K	664.31	Joback Method
cpg	349.42	J/mol×K	629.07	Joback Method
cpg	337.02	J/mol×K	593.82	Joback Method
cpg	392.43	J/mol×K	770.06	Joback Method
dvisc	0.0001728	Pa×s	558.57	Joback Method
dvisc	0.0002153	Pa×s	521.44	Joback Method
dvisc	0.0002774	Pa×s	484.31	Joback Method
dvisc	0.0003728	Pa×s	447.18	Joback Method
dvisc	0.0005287	Pa×s	410.05	Joback Method
dvisc	0.0008036	Pa×s	372.92	Joback Method
dvisc	0.0013400	Pa×s	335.79	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C3686553&Units=SI
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

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

Latest version available from:

https://www.chemeo.com/cid/15-620-6/Benzoic-acid-2-ethoxy-methyl-ester.pdf

Generated by Cheméo on 2024-04-26 06:37:19.485818614 +0000 UTC m=+16402688.406395925.

Cheméo (https://www.chemeo.com) is the biggest free database of chemical and physical data for the process industry.