

Benzoic acid, 2-methoxy-, ethyl ester

Other names:	o-Anisic acid, ethyl ester Ethyl o-methoxybenzoate Ethyl 2-methoxybenzoate o-Methoxybenzoic acid, ethyl ester ethyl o-anisate
Inchi:	InChI=1S/C10H12O3/c1-3-13-10(11)8-6-4-5-7-9(8)12-2/h4-7H,3H2,1-2H3
InchiKey:	FNODWEPAWIJGPM-UHFFFAOYSA-N
Formula:	C10H12O3
SMILES:	CCOC(=O)c1ccccc1OC
Mol. weight [g/mol]:	180.20
CAS:	7335-26-4

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	1412.10		NIST Webbook
rinpol	1435.00		NIST Webbook
rinpol	1412.10		NIST Webbook
tb	534.65 ± 1.00	K	NIST Webbook
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/molxK	558.57	Joback Method

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

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	408.20	K	1.60	NIST Webbook

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=C7335264&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
tbrp:	Boiling point at reduced pressure
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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