

Benzene, 2-ethoxy-1,3-dimethoxy-

Other names:	2-Ethoxy-1,3-dimethoxybenzene Ethylsyringol 2,6-Dimethoxyphenetole
Inchi:	InChI=1S/C10H14O3/c1-4-13-10-8(11-2)6-5-7-9(10)12-3/h5-7H,4H2,1-3H3
InchiKey:	COPJTXDDUKMXHR-UHFFFAOYSA-N
Formula:	C10H14O3
SMILES:	CCOc1c(OC)cccc1OC
Mol. weight [g/mol]:	182.22
CAS:	29515-37-5

Physical Properties

Property code	Value	Unit	Source
gf	-188.53	kJ/mol	Joback Method
hf	-432.80	kJ/mol	Joback Method
hfus	18.48	kJ/mol	Joback Method
hvap	48.68	kJ/mol	Joback Method
log10ws	-2.25		Crippen Method
logp	2.103		Crippen Method
mcvol	145.610	ml/mol	McGowan Method
pc	2690.21	kPa	Joback Method
rinpol	1533.00		NIST Webbook
rinpol	1533.70		NIST Webbook
tb	532.10	K	Joback Method
tc	734.18	K	Joback Method
tf	320.61	K	Joback Method
vc	0.541	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	330.29	J/mol×K	532.10	Joback Method
cpg	343.78	J/mol×K	565.78	Joback Method
cpg	356.77	J/mol×K	599.46	Joback Method
cpg	369.24	J/mol×K	633.14	Joback Method

cpg	381.17	J/molxK	666.82	Joback Method
cpg	392.54	J/molxK	700.50	Joback Method
cpg	403.34	J/molxK	734.18	Joback Method
dvisc	0.0008685	Paxs	320.61	Joback Method
dvisc	0.0005382	Paxs	355.86	Joback Method
dvisc	0.0003635	Paxs	391.11	Joback Method
dvisc	0.0002620	Paxs	426.36	Joback Method
dvisc	0.0001985	Paxs	461.60	Joback Method
dvisc	0.0001565	Paxs	496.85	Joback Method
dvisc	0.0001273	Paxs	532.10	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C29515375&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Joback Method:	https://en.wikipedia.org/wiki/Joback_method

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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