Anethole

Other names:	1-(p-Methoxyphenyl)propene
	1-Methoxy-4-(1-propenyl)benzene
	1-Methoxy-4-propenylbenzene
	1-Propene, 1-(4-methoxyphenyl)-
	4-(1-Propenyl)anisole
	4-Methoxy-1-propenylbenzene
	4-Methoxypropenylbenzene
	4-Propenylanisole
	Anethol
	Anise camphor
	Aniskampfer
	Anisole, p-propenyl-
	Benzene, 1-methoxy-4-(1-propen-1-yl)-
	Benzene, 1-methoxy-4-(1-propenyl)-
	Isoestragole
	Methoxy-4-propenylbenzene
	Monasirup
	NSC 4018
	Nauli "gum"
	Nauli gum
	Oil of aniseed
	Propene, 1-(p-methoxyphenyl)-
	p-(1-Propenyl)anisole
	p-Anethole
	p-Methoxy-«beta»-methylstyrene
	p-Methoxy-Â«betaÂ»-methylstyrene
	p-Propenylanisole
	p-Propenylphenyl methyl ether
Inchi:	InChI=1S/C10H12O/c1-3-4-9-5-7-10(11-2)8-6-9/h3-8H,1-2H3
InchiKey:	RUVINXPYWBROJD-UHFFFAOYSA-N
Formula:	C10H12O
SMILES:	CC=Cc1ccc(OC)cc1
Mol. weight [g/mol]:	148.20
CAS:	104-46-1

Physical Properties

Property code	Value	Unit	Source

chl	-5544.55	kJ/mol	NIST Webbook
gf	111.32	kJ/mol	Joback Method
hf	-39.67	kJ/mol	Joback Method
hfus	16.70	kJ/mol	Joback Method
hvap	61.90	kJ/mol	NIST Webbook
log10ws	-2.83		Crippen Method
logp	2.728		Crippen Method
mcvol	129.570	ml/mol	McGowan Method
pc	2995.87	kPa	Joback Method
rinpol	1288.00		NIST Webbook
rinpol	1269.00		NIST Webbook
rinpol	1251.00		NIST Webbook
rinpol	1283.00		NIST Webbook
rinpol	1286.00		NIST Webbook
rinpol	1285.00		NIST Webbook
rinpol	1257.00		NIST Webbook
rinpol	1257.00		NIST Webbook
rinpol	1251.00		NIST Webbook
rinpol	1289.30		NIST Webbook
rinpol	1283.50		NIST Webbook
rinpol	1264.00		NIST Webbook
rinpol	1279.00		NIST Webbook
ripol	1847.00		NIST Webbook
ripol	1819.00		NIST Webbook
ripol	1822.00		NIST Webbook
ripol	1808.00		NIST Webbook
ripol	1815.00		NIST Webbook
ripol	1809.00		NIST Webbook
ripol	1817.00		NIST Webbook
ripol	1834.00		NIST Webbook
tb	506.00 ± 4.00	K	NIST Webbook
tb	508.00	K	NIST Webbook
tc	700.83	K	Joback Method
tf	295.00 ± 0.50	K	NIST Webbook
vc	0.485	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	264.61	J/mol×K	486.44	Joback Method

cpg	278.48	J/mol×K	522.17	Joback Method
cpg	291.59	J/mol×K	557.90	Joback Method
cpg	303.96	J/mol×K	593.63	Joback Method
cpg	315.63	J/mol×K	629.36	Joback Method
cpg	326.61	J/mol×K	665.09	Joback Method
cpg	336.94	J/mol×K	700.83	Joback Method
dvisc	0.0017616	Pa×s	258.55	Joback Method
dvisc	0.0009103	Pa×s	296.53	Joback Method
dvisc	0.0005465	Pa×s	334.51	Joback Method
dvisc	0.0003641	Pa×s	372.50	Joback Method
dvisc	0.0002615	Pa×s	410.48	Joback Method
dvisc	0.0001986	Pa×s	448.46	Joback Method
dvisc	0.0001575	Pa×s	486.44	Joback Method

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/T + C*ln(T) + D*T^2
Coeff. A	9.42264e+01
Coeff. B	-1.06388e+04
Coeff. C	-1.11978e+01
Coeff. D	4.15545e-06
Temperature range (K), min.	294.50
Temperature range (K), max.	723.00

Sources

McGowan Method: http://link.springer.com/article/10.1007/BF02311772

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C104461&Units=SI

KDB Vapor Pressure Data: https://www.cheric.org/research/kdb/hcprop/showprop.php?cmpid=1030

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

Legend

chl:	Standard liquid enthalpy of combustion
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
pvap:	Vapor pressure
rinpol:	Non-polar retention indices
ripol:	Polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume