

Anethole

Other names: (E)-1-(4-methoxyphenyl)propene
(E)-1-Methoxy-4(1-propenyl)benzene
(E)-1-p-methoxyphenylpropene
(E)-4-propenylanisole
(E)-Anethol
(E)-Anethole
(E)-Anetole
Anethole (E)
E-trans-Anethole
anethole, trans-
benzene, 1-methoxy-4-(1-propenyl)-, trans-
trans-1-(4-methoxyphenyl)-1-propene
trans-1-(p-methoxyphenyl)propene
trans-1-methoxy-4-(1-propenyl)benzene
trans-1-p-anisylpropene
trans-4-(1-propenyl)anisole
trans-Anethol
trans-anethole
trans-p-anethole
trans-p-methoxy-.beta.-methylstyrene

Inchi: InChI=1S/C10H12O/c1-3-4-9-5-7-10(11-2)8-6-9/h3-8H,1-2H3/b4-3+

InchiKey: RUVINXPYWBROJD-ONEGZZNKSA-N

Formula: C10H12O

SMILES: CC=Cc1ccc(OC)cc1

Mol. weight [g/mol]: 148.20

CAS: 4180-23-8

Physical Properties

Property code	Value	Unit	Source
gf	111.32	kJ/mol	Joback Method
hf	-39.67	kJ/mol	Joback Method
hfus	16.70	kJ/mol	Joback Method
hvap	43.16	kJ/mol	Joback Method
log10ws	-2.83		Crippen Method
logp	2.728		Crippen Method
mcvol	129.570	ml/mol	McGowan Method
pc	2995.87	kPa	Joback Method

rinpol	1283.00	NIST Webbook
rinpol	1284.00	NIST Webbook
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ripol	1809.00		NIST Webbook
ripol	1809.00		NIST Webbook
ripol	1827.00		NIST Webbook
ripol	1809.00		NIST Webbook
tb	508.50 ± 1.00	K	NIST Webbook
tb	508.70	K	NIST Webbook
tb	508.85 ± 0.70	K	NIST Webbook
tc	700.83	K	Joback Method
tf	258.55	K	Joback Method
vc	0.485	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	336.94	J/mol×K	700.83	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	264.61	J/mol×K	486.44	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
hvapt	78.30	kJ/mol	348.00	NIST Webbook

pvap	0.08	kPa	331.50	Vaporization thermodynamics of compounds modeling lignin structural units
pvap	0.07	kPa	328.40	Vaporization thermodynamics of compounds modeling lignin structural units
pvap	0.06	kPa	326.40	Vaporization thermodynamics of compounds modeling lignin structural units
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pvap	0.04	kPa	321.40	Vaporization thermodynamics of compounds modeling lignin structural units
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pvap	0.02	kPa	308.40	Vaporization thermodynamics of compounds modeling lignin structural units
pvap	0.01	kPa	304.40	Vaporization thermodynamics of compounds modeling lignin structural units
pvap	7.74e-03	kPa	300.40	Vaporization thermodynamics of compounds modeling lignin structural units

pvap	5.67e-03	kPa	296.50	Vaporization thermodynamics of compounds modeling lignin structural units
pvap	0.09	kPa	333.40	Vaporization thermodynamics of compounds modeling lignin structural units

Sources

Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Fluid phase equilibria and mass transfer studies applied to supercritical fluid extraction thermodynamics of compounds modeling lignin structural units	https://www.doi.org/10.1016/j.fluid.2016.02.042
Joback Method:	https://www.doi.org/10.1016/j.fluid.2019.03.004
McGowan Method:	https://en.wikipedia.org/wiki/Joback_method
NIST Webbook:	http://link.springer.com/article/10.1007/BF02311772
Crippen Method:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C4180238&Units=SI
	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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
hvapt:	Enthalpy of vaporization at a given temperature
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

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