(E)-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)-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
	Anethole
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:	C/C=C/c1ccc(OC)cc1
Mol. weight [g/mol]:	148.21
CAS:	4180-23-8

Physical Properties

Property code	Value	Unit	Source
hf	-21.13	kJ/mol	Cheméo Relay (1.0)
hfus	16.70	kJ/mol	Joback Method
hvap	60.27	kJ/mol	Cheméo Relay (1.0)
ie	7.70	eV	Cheméo Relay (1.0)
log10ws	-3.60		Cheméo Relay (1.0)
logp	2.728		Crippen Method
mcvol	129.570	ml/mol	McGowan Method
pc	2995.87	kPa	Joback Method

rinpol	1288.00	NIST Webbook
rinpol	1283.00	NIST Webbook
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ripol	1838.00		NIST Webbook
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tb	508.50 ± 1.00	K	NIST Webbook
tb	508.85 ± 0.70	K	NIST Webbook
tb	508.70	K	NIST Webbook
tc	705.71	K	Cheméo Relay (1.0)
tf	294.80	K	Jean-Claude Bradley Open Melting Point Dataset (2014, CC0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
hvapt	78.30	kJ/mol	348.00	NIST Webbook
pvap	0.03	kPa	316.40	Vaporization thermodynamics of compounds modeling lignin structural units
pvap	0.04	kPa	321.40	Vaporization thermodynamics of compounds modeling lignin structural units
pvap	0.02	kPa	308.40	Vaporization thermodynamics of compounds modeling lignin structural units
pvap	0.02	kPa	312.30	Vaporization thermodynamics of compounds modeling lignin structural units
pvap	0.02	kPa	313.20	Vaporization thermodynamics of compounds modeling lignin structural units
pvap	5.67e-03	kPa	296.50	Vaporization thermodynamics of compounds modeling lignin structural units
pvap	0.03	kPa	318.50	Vaporization thermodynamics of compounds modeling lignin structural units
pvap	0.01	kPa	304.40	Vaporization thermodynamics of compounds modeling lignin structural units
pvap	0.05	kPa	323.40	Vaporization thermodynamics of compounds modeling lignin structural units
pvap	0.06	kPa	326.40	Vaporization thermodynamics of compounds modeling lignin structural units

pvap	0.07	kPa	328.40	Vaporization thermodynamics of compounds modeling lignin structural units
pvap	0.08	kPa	331.50	Vaporization thermodynamics of compounds modeling lignin structural units
pvap	0.09	kPa	333.40	Vaporization thermodynamics of compounds modeling lignin structural units
pvap	7.74e-03	kPa	300.40	Vaporization thermodynamics of compounds modeling lignin structural units

Correlations

Information	Value
Property code	cpg
Equation	$Y = A + B \cdot T + C \cdot T^2 + D \cdot T^3 + E \cdot T.$
Y unit	J/mol×K
Coeff. A	-1.44900e+01
Coeff. B	7.72240e-01
Coeff. C	-4.57160e-04
Coeff. D	1.01000e-07
Coeff. E	0.00000e+00
Basis	predicted
Temperature range (K), min.	273.00
Temperature range (K), max.	1000.00

Information	Value
Property code	dvisc
Equation	Y = exp(A + B/T + C·ln(T) + D·T^E)
Y unit	Pa×s
Coeff. A	-1.14954e+01
Coeff. B	1.33253e+03
Coeff. C	0.00000e+00
Coeff. D	0.00000e+00
Coeff. E	0.00000e+00
Basis	predicted

Comment	Liquid phase. Joback/Reid (1987), valid from Tf to 0.7·Tc.
Temperature range (K), min.	294.80
Temperature range (K), max.	490.78

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Cheméo Relay (1.0):	
Cheméo Relay (1.0, beta):	
Jean-Claude Bradley Open Melting Point Dataset (2014, CC0):	https://figshare.com/articles/Jean_Claude_Bradley_Open_Melting_Point_Datset/1031637
Vaporization thermodynamics of compounds modeling lignin structural units:	https://www.doi.org/10.1016/j.fluid.2019.03.004
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C4180238&Units=SI
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
Fluid phase equilibria and mass transfer studies applied to supercritical fluid extraction of Illicium verum volatile oil:	https://www.doi.org/10.1016/j.fluid.2016.02.042
Joback Method:	https://en.wikipedia.org/wiki/Joback_method

Legend

cpg:	Ideal gas heat capacity
dvisc:	Dynamic viscosity
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
ie:	Ionization energy
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

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