

cis-Anethole

Other names:	cis-Anethol (Z)-Anethole (Z)-Anethol
Inchi:	InChI=1S/C10H12O/c1-3-4-9-5-7-10(11-2)8-6-9/h3-8H,1-2H3/b4-3-
InchiKey:	RUVINXPYWBROJD-ARJAWSKDSA-N
Formula:	C10H12O
SMILES:	CC=Cc1ccc(OC)cc1
Mol. weight [g/mol]:	148.20
CAS:	25679-28-1

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	1245.00		NIST Webbook
rinpol	1256.70		NIST Webbook
rinpol	1267.00		NIST Webbook
rinpol	1220.00		NIST Webbook
rinpol	1241.00		NIST Webbook
rinpol	1241.00		NIST Webbook
rinpol	1269.00		NIST Webbook
rinpol	1262.00		NIST Webbook
rinpol	1209.00		NIST Webbook
rinpol	1209.00		NIST Webbook
rinpol	1267.00		NIST Webbook
rinpol	1258.00		NIST Webbook
rinpol	1209.00		NIST Webbook
rinpol	1252.00		NIST Webbook
rinpol	1215.00		NIST Webbook
rinpol	1256.70		NIST Webbook
rinpol	1216.00		NIST Webbook

rinpol	1254.00		NIST Webbook
rinpol	1258.00		NIST Webbook
rinpol	1233.00		NIST Webbook
rinpol	1257.00		NIST Webbook
rinpol	1254.00		NIST Webbook
rinpol	1230.00		NIST Webbook
rinpol	1223.00		NIST Webbook
rinpol	1220.00		NIST Webbook
rinpol	1262.00		NIST Webbook
ripol	1759.00		NIST Webbook
ripol	1800.00		NIST Webbook
ripol	1780.00		NIST Webbook
ripol	1759.00		NIST Webbook
ripol	1732.00		NIST Webbook
ripol	1746.00		NIST Webbook
ripol	1759.00		NIST Webbook
tb	486.44	K	Joback Method
tc	700.83	K	Joback Method
tf	258.55	K	Joback Method
vc	0.485	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	264.61	J/molxK	486.44	Joback Method
cpg	278.48	J/molxK	522.17	Joback Method
cpg	291.59	J/molxK	557.90	Joback Method
cpg	303.96	J/molxK	593.63	Joback Method
cpg	315.63	J/molxK	629.36	Joback Method
cpg	326.61	J/molxK	665.09	Joback Method
cpg	336.94	J/molxK	700.83	Joback Method
dvisc	0.0017616	Paxs	258.55	Joback Method
dvisc	0.0009103	Paxs	296.53	Joback Method
dvisc	0.0005465	Paxs	334.51	Joback Method
dvisc	0.0003641	Paxs	372.50	Joback Method
dvisc	0.0002615	Paxs	410.48	Joback Method
dvisc	0.0001986	Paxs	448.46	Joback Method
dvisc	0.0001575	Paxs	486.44	Joback Method
hvapt	68.70	kJ/mol	348.00	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=C25679281&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
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
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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