ANISYL ALCOHOL

Other names:	Benzyl alcohol, p-methoxy-
	p-Anisyl alcohol
	p-Methoxybenzyl alcohol
	Anise alcohol
	Anisic alcohol
	4-Methoxybenzyl alcohol
	Anisyl alcohol
	p-Anisol alcohol
	4-Methoxybenzenemethanol
	Anis alcohol
	4-Anisylalcohol
	4-(Hydroxymethyl)anisole
	NSC 2151
Inchi:	InChI=1S/C8H10O2/c1-10-8-4-2-7(6-9)3-5-8/h2-5,9H,6H2,1H3
InchiKey:	MSHFRERJPWKJFX-UHFFFAOYSA-N
Formula:	C8H10O2
SMILES:	COc1ccc(CO)cc1
Mol. weight [g/mol]:	138.17

Physical Properties

Property code	Value	Unit	Source
hf	-257.04	kJ/mol	Cheméo Relay (1.0)
hfus	15.40	kJ/mol	Joback Method
hvap	78.50	kJ/mol	Cheméo Relay (1.0)
ie	8.21	eV	Cheméo Relay (1.0)
log10ws	-1.32		Cheméo Relay (1.0)
logp	1.188		Crippen Method
mcvol	111.560	ml/mol	McGowan Method
pc	3930.78	kPa	Joback Method
rinpol	1242.00		NIST Webbook
rinpol	1293.00		NIST Webbook
rinpol	1277.00		NIST Webbook
rinpol	1279.00		NIST Webbook
rinpol	1279.00		NIST Webbook
rinpol	1279.00		NIST Webbook
rinpol	1282.00		NIST Webbook
rinpol	1270.00		NIST Webbook

rinpol	1308.00		NIST Webbook
rinpol	1303.00		NIST Webbook
rinpol	1304.00		NIST Webbook
rinpol	1304.00		NIST Webbook
rinpol	1312.00		NIST Webbook
rinpol	1307.00		NIST Webbook
rinpol	1284.00		NIST Webbook
rinpol	1290.00		NIST Webbook
rinpol	1278.00		NIST Webbook
rinpol	1242.00		NIST Webbook
rinpol	1244.00		NIST Webbook
rinpol	1244.00		NIST Webbook
rinpol	1249.00		NIST Webbook
rinpol	1295.00		NIST Webbook
rinpol	1290.00		NIST Webbook
rinpol	1267.00		NIST Webbook
rinpol	1295.00		NIST Webbook
rinpol	1275.00		NIST Webbook
rinpol	1267.00		NIST Webbook
rinpol	1277.00		NIST Webbook
rinpol	1273.00		NIST Webbook
rinpol	1246.80		NIST Webbook
rinpol	1273.00		NIST Webbook
rinpol	1279.00		NIST Webbook
ripol	2302.00		NIST Webbook
ripol	2305.00		NIST Webbook
ripol	2268.00		NIST Webbook
ripol	2290.00		NIST Webbook
ripol	2305.00		NIST Webbook
ripol	2290.00		NIST Webbook
tb	532.30	K	NIST Webbook
tb	489.15 ± 2.00	K	NIST Webbook
tc	733.27	K	Cheméo Relay (1.0)
tf	290.15 ± 1.50	K	NIST Webbook

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	245.43	J/mol×K	528.70	Joback Method
cpg	255.61	J/mol×K	561.54	Joback Method
cpg	265.29	J/mol×K	594.39	Joback Method

cpg	274.50	J/mol×K	627.23	Joback Method
cpg	283.23	J/mol×K	660.07	Joback Method
cpg	291.49	J/mol×K	692.92	Joback Method
cpg	299.29	J/mol×K	725.76	Joback Method
dvisc	0.0063822	Pa×s	301.91	Joback Method
dvisc	0.0022019	Pa×s	339.71	Joback Method
dvisc	0.0009401	Pa×s	377.51	Joback Method
dvisc	0.0004686	Pa×s	415.31	Joback Method
dvisc	0.0002624	Pa×s	453.10	Joback Method
dvisc	0.0001606	Pa×s	490.90	Joback Method
dvisc	0.0001055	Pa×s	528.70	Joback Method
hvapt	95.60	kJ/mol	409.00	NIST Webbook
hvapt	71.70	kJ/mol	403.50	NIST Webbook

Sources

Cheméo Relay (1.0, beta):

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C105135&Units=SI

Joback Method: https://en.wikipedia.org/wiki/Joback_method

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

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):

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
rinpol: Non-polar retention indices

ripol:	Polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point