o-Isopropylanisole

Other names:	Anisole, o-isopropyl-
	Benzene, 1-methoxy-2-(1-methylethyl)-
	2-(o-Methoxyphenyl)propane
Inchi:	InChI=1S/C10H14O/c1-8(2)9-6-4-5-7-10(9)11-3/h4-8H,1-3H3
InchiKey:	NNZRVXTXKISCGS-UHFFFAOYSA-N
Formula:	C10H14O
SMILES:	COc1ccccc1C(C)C
Mol. weight [g/mol]:	150.22
CAS:	2944-47-0

Physical Properties

Property code	Value	Unit	Source
gf	28.66	kJ/mol	Joback Method
hf	-162.17	kJ/mol	Joback Method
hfus	12.97	kJ/mol	Joback Method
hvap	42.81	kJ/mol	Joback Method
log10ws	-2.78		Crippen Method
logp	2.819		Crippen Method
mcvol	133.870	ml/mol	McGowan Method
pc	2856.62	kPa	Joback Method
rinpol	1118.00		NIST Webbook
rinpol	1118.00		NIST Webbook
tb	481.84	K	Joback Method
tc	690.94	K	Joback Method
tf	248.63	K	Joback Method
vc	0.499	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	281.84	J/mol×K	481.84	Joback Method
cpg	296.54	J/mol×K	516.69	Joback Method
cpg	310.53	J/mol×K	551.54	Joback Method
cpg	323.81	J/mol×K	586.39	Joback Method

cpg	336.41	J/mol×K	621.24	Joback Method
cpg	348.34	J/mol×K	656.09	Joback Method
cpg	359.60	J/mol×K	690.94	Joback Method
dvisc	0.0026779	Pa×s	248.63	Joback Method
dvisc	0.0012548	Pa×s	287.50	Joback Method
dvisc	0.0007043	Pa×s	326.37	Joback Method
dvisc	0.0004470	Pa×s	365.24	Joback Method
dvisc	0.0003097	Pa×s	404.10	Joback Method
dvisc	0.0002288	Pa×s	442.97	Joback Method
dvisc	0.0001775	Pa×s	481.84	Joback Method

Sources

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
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C2944470&Units=SI

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
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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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