Anisole, 3-ethyl-5-methyl

Inchi: InChI=1S/C10H14O/c1-4-9-5-8(2)6-10(7-9)11-3/h5-7H,4H2,1-3H3
InchiKey: SMOHZTWJKGTUIA-UHFFFAOYSA-N
Formula: C10H14O
SMILES: CCc1cc(C)cc(OC)c1
Mol. weight [g/mol]: 150.22

Physical Properties

Property code	Value	Unit	Source
gf	21.47	kJ/mol	Joback Method
hf	-168.36	kJ/mol	Joback Method
hfus	16.11	kJ/mol	Joback Method
hvap	43.86	kJ/mol	Joback Method
log10ws	-2.87		Crippen Method
logp	2.566		Crippen Method
mcvol	133.870	ml/mol	McGowan Method
pc	2787.66	kPa	Joback Method
rinpol	1179.00		NIST Webbook
rinpol	1179.00		NIST Webbook
rinpol	1204.00		NIST Webbook
tb	487.26	K	Joback Method
tc	692.88	K	Joback Method
tf	276.15	K	Joback Method
vc	0.505	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	282.14	J/mol×K	487.26	Joback Method
cpg	296.04	J/mol×K	521.53	Joback Method
cpg	309.33	J/mol×K	555.80	Joback Method
cpg	322.01	J/mol×K	590.07	Joback Method
cpg	334.09	J/mol×K	624.34	Joback Method
cpg	345.58	J/mol×K	658.61	Joback Method
cpg	356.48	J/mol×K	692.88	Joback Method

dvisc	0.0013933	Pa×s	276.15	Joback Method
dvisc	0.0008168	Pa×s	311.33	Joback Method
dvisc	0.0005336	Pa×s	346.52	Joback Method
dvisc	0.0003771	Pa×s	381.70	Joback Method
dvisc	0.0002826	Pa×s	416.89	Joback Method
dvisc	0.0002215	Pa×s	452.07	Joback Method
dvisc	0.0001798	Pa×s	487.26	Joback Method

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=R142724&Units=SI
Crippen Method:	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
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