2,6-DIMETHYLANISOLE

Other names: 2,6-Dimethylanisole
Inchi: InChI=1S/C9H12O/c1-7-5-4-6-8(2)9(7)10-3/h4-6H,1-3H3
InchiKey: GFNZJAUVJCGWLW-UHFFFAOYSA-N
Formula: C9H12O
SMILES: COc1c(C)cccc1C
Mol. weight [g/mol]: 136.19

Physical Properties

Property code	Value	Unit	Source
af	0.4211		Cheméo Relay (1.0)
gf	13.05	kJ/mol	Joback Method
hf	-134.47	kJ/mol	Cheméo Relay (1.0)
hfus	13.52	kJ/mol	Joback Method
hvap	52.37	kJ/mol	Cheméo Relay (1.0)
ie	8.10 ± 0.02	eV	NIST Webbook
ie	8.51	eV	NIST Webbook
ie	8.53	eV	NIST Webbook
log10ws	-2.26		Cheméo Relay (1.0)
logp	2.312		Crippen Method
mcvol	119.780	ml/mol	McGowan Method
pc	3093.29	kPa	Joback Method
rinpol	1040.00		NIST Webbook
rinpol	1062.00		NIST Webbook
rinpol	1078.00		NIST Webbook
rinpol	1062.00		NIST Webbook
tb	455.70	K	NIST Webbook
tc	671.39	K	Cheméo Relay (1.0)
tf	243.33	K	Cheméo Relay (1.0)
vc	0.430	m3/kmol	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	239.84	J/mol×K	464.38	Joback Method

cpg	252.59	J/mol×K	499.13	Joback Method
cpg	264.78	J/mol×K	533.88	Joback Method
cpg	276.44	J/mol×K	568.63	Joback Method
cpg	287.55	J/mol×K	603.38	Joback Method
cpg	298.13	J/mol×K	638.13	Joback Method
cpg	308.18	J/mol×K	672.88	Joback Method
dvisc	0.0013208	Pa×s	264.88	Joback Method
dvisc	0.0007933	Pa×s	298.13	Joback Method
dvisc	0.0005277	Pa×s	331.38	Joback Method
dvisc	0.0003782	Pa×s	364.63	Joback Method
dvisc	0.0002865	Pa×s	397.88	Joback Method
dvisc	0.0002266	Pa×s	431.13	Joback Method
dvisc	0.0001853	Pa×s	464.38	Joback Method

Sources

Cheméo Relay (1.0):

Cheméo Relay (1.0, beta):

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C1004666&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

Legend

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