2,3,6-Trimethylanisole

Other names: Anisole, 2,3,6-trimethyl-
2,3,6-Trimethylanisole
Inchi: InChI=1S/C10H14O/c1-7-5-6-8(2)10(11-4)9(7)3/h5-6H,1-4H3
InchiKey: MIOQAXCZXWHELT-UHFFFAOYSA-N
Formula: C10H14O
SMILES: COc1c(C)ccc(C)c1C
Mol. weight [g/mol]: 150.22

Physical Properties

Property code	Value	Unit	Source
hf	-163.69	kJ/mol	Cheméo Relay (1.0)
hfus	15.72	kJ/mol	Joback Method
hvap	58.69	kJ/mol	Cheméo Relay (1.0)
ie	7.85	eV	Cheméo Relay (1.0)
logp	2.620		Crippen Method
mcvol	133.870	ml/mol	McGowan Method
rinpol	1163.00		NIST Webbook
tb	481.18	K	Cheméo Relay (1.0)
tf	269.30	K	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	282.49	J/mol×K	492.24	Joback Method
cpg	296.02	J/mol×K	526.72	Joback Method
cpg	308.99	J/mol×K	561.19	Joback Method
cpg	321.42	J/mol×K	595.67	Joback Method
cpg	333.28	J/mol×K	630.14	Joback Method
cpg	344.60	J/mol×K	664.62	Joback Method
cpg	355.37	J/mol×K	699.09	Joback Method
dvisc	0.0010441	Pa×s	288.67	Joback Method
dvisc	0.0006612	Pa×s	322.60	Joback Method
dvisc	0.0004568	Pa×s	356.53	Joback Method
dvisc	0.0003365	Pa×s	390.46	Joback Method

dvisc	0.0002603	Pa×s	424.38	Joback Method
dvisc	0.0002092	Pa×s	458.31	Joback Method
dvisc	0.0001732	Pa×s	492.24	Joback Method

Sources

Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws
Cheméo Relay (1.0):
Cheméo Relay (1.0, beta):
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C21573364&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

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
ie: Ionization energy
logp: Octanol/Water partition coefficient
mcvol: McGowan's characteristic volume
rinpol: Non-polar retention indices
tb: Normal Boiling Point Temperature
tf: Normal melting (fusion) point

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