METHYL 3-METHOXY-4-ETHOXYBENZOATE

Inchi: InChI=1S/C11H14O4/c1-4-15-9-6-5-8(11(12)14-3)7-10(9)13-2/h5-7H,4H2,1-3H3
InchiKey: HVLQOCXAZMSAPT-UHFFFAOYSA-N
Formula: C11H14O4
SMILES: CCOc1ccc(C(=O)OC)cc1OC
Mol. weight [g/mol]: 210.23

Physical Properties

Property code	Value	Unit	Source
af	0.6744		Cheméo Relay (1.0)
hf	-621.35	kJ/mol	Cheméo Relay (1.0)
hfus	22.67	kJ/mol	Joback Method
hvap	77.67	kJ/mol	Cheméo Relay (1.0)
ie	8.35	eV	Cheméo Relay (1.0)
log10ws	-2.85		Cheméo Relay (1.0)
logp	1.881		Crippen Method
mcvol	161.270	ml/mol	McGowan Method
pc	2600.43	kPa	Joback Method
rinpol	1520.00		NIST Webbook
rinpol	1520.00		NIST Webbook
tb	564.77	K	Cheméo Relay (1.0)
tc	749.96	K	Cheméo Relay (1.0)
tf	354.22	K	Cheméo Relay (1.0)
vc	0.605	m3/kmol	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	394.96	J/mol×K	608.85	Joback Method
cpg	408.45	J/mol×K	643.33	Joback Method
cpg	421.30	J/mol×K	677.82	Joback Method
cpg	433.48	J/mol×K	712.30	Joback Method
cpg	444.99	J/mol×K	746.78	Joback Method
cpg	455.79	J/mol×K	781.27	Joback Method
cpg	465.87	J/mol×K	815.75	Joback Method

dvisc	0.0007937	Pa×s	381.81	Joback Method
dvisc	0.0005080	Pa×s	419.65	Joback Method
dvisc	0.0003500	Pa×s	457.49	Joback Method
dvisc	0.0002553	Pa×s	495.33	Joback Method
dvisc	0.0001948	Pa×s	533.17	Joback Method
dvisc	0.0001540	Pa×s	571.01	Joback Method
dvisc	0.0001254	Pa×s	608.85	Joback Method

Sources

Cheméo Relay (1.0, beta):

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C3535248&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

af: Acentric Factor
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
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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