4-ETHOXY-3-METHOXYBENZALDEHYDE

Other names: 4-Ethoxy-m-anisaldehyde
Benzaldehyde, 4-ethoxy-3-methoxy-
Inchi: InChI=1S/C10H12O3/c1-3-13-9-5-4-8(7-11)6-10(9)12-2/h4-7H,3H2,1-2H3
InchiKey: BERFDQAMXIBOHM-UHFFFAOYSA-N
Formula: C10H12O3
SMILES: CCOc1ccc(C=O)cc1OC
Mol. weight [g/mol]: 180.20

Physical Properties

Property code	Value	Unit	Source
hfus	19.58	kJ/mol	Joback Method
hvap	71.15	kJ/mol	Cheméo Relay (1.0)
ie	8.55	eV	Cheméo Relay (1.0)
log10ws	-2.19		Aqueous Solubility Prediction Method
logp	1.906		Crippen Method
mcvol	141.310	ml/mol	McGowan Method
tb	554.22	K	Cheméo Relay (1.0)
tf	335.90	K	Aqueous Solubility Prediction Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	324.53	J/mol×K	558.34	Joback Method
cpg	336.96	J/mol×K	592.94	Joback Method
cpg	348.82	J/mol×K	627.54	Joback Method
cpg	360.10	J/mol×K	662.14	Joback Method
cpg	370.79	J/mol×K	696.75	Joback Method
cpg	380.90	J/mol×K	731.35	Joback Method
cpg	390.40	J/mol×K	765.95	Joback Method
dvisc	0.0011812	Pa×s	340.38	Joback Method
dvisc	0.0007465	Pa×s	376.71	Joback Method
dvisc	0.0005114	Pa×s	413.03	Joback Method

dvisc	0.0003725	Pa×s	449.36	Joback Method
dvisc	0.0002845	Pa×s	485.69	Joback Method
dvisc	0.0002255	Pa×s	522.01	Joback Method
dvisc	0.0001843	Pa×s	558.34	Joback Method

Sources

Cheméo Relay (1.0):

Cheméo Relay (1.0, beta):

Aqueous Solubility Prediction Method: http://onschallenge.wikispaces.com/file/view/AqueousDataset002.xlsx/351826032/AqueousDa

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C120252&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
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
tb: Normal Boiling Point Temperature
tf: Normal melting (fusion) point