4-Ethoxy-3-anisaldehyde

Other names:	4-Ethoxy-3-methoxybenzaldehyde
	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
CAS:	120-25-2

Physical Properties

Property code	Value	Unit	Source
gf	-183.05	kJ/mol	Joback Method
hf	-386.16	kJ/mol	Joback Method
hfus	19.58	kJ/mol	Joback Method
hvap	52.99	kJ/mol	Joback Method
log10ws	-2.19		Aqueous Solubility Prediction Method
logp	1.906		Crippen Method
mcvol	141.310	ml/mol	McGowan Method
pc	2963.34	kPa	Joback Method
tb	558.34	K	Joback Method
tc	765.95	K	Joback Method
tf	335.90	K	Aqueous Solubility Prediction Method
vc	0.540	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	324.53	J/mol×K	558.34	Joback Method
cpg	380.90	J/mol×K	731.35	Joback Method
cpg	370.79	J/mol×K	696.75	Joback Method
cpg	360.10	J/mol×K	662.14	Joback Method

cpg	348.82	J/mol×K	627.54	Joback Method
cpg	336.96	J/mol×K	592.94	Joback Method
cpg	390.40	J/mol×K	765.95	Joback Method
dvisc	0.0001843	Pa×s	558.34	Joback Method
dvisc	0.0002255	Pa×s	522.01	Joback Method
dvisc	0.0002845	Pa×s	485.69	Joback Method
dvisc	0.0003725	Pa×s	449.36	Joback Method
dvisc	0.0005114	Pa×s	413.03	Joback Method
dvisc	0.0007465	Pa×s	376.71	Joback Method
dvisc	0.0011812	Pa×s	340.38	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C120252&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
Aqueous Solubility Prediction Method:	http://onschallenge.wikispaces.com/file/view/AqueousDataset002.xlsx/351826032/AqueousDa

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

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