

2,5-Dimethoxy-4-propoxybenzaldehyde

Inchi:	InChI=1S/C12H16O4/c1-4-5-16-12-7-10(14-2)9(8-13)6-11(12)15-3/h6-8H,4-5H2,1-3H3
InchiKey:	QSBRRZLPYAVNF-UHFFFAOYSA-N
Formula:	C12H16O4
SMILES:	CCCOc1cc(OC)c(C=O)cc1OC
Mol. weight [g/mol]:	224.25

Physical Properties

Property code	Value	Unit	Source
gf	-280.84	kJ/mol	Joback Method
hf	-571.13	kJ/mol	Joback Method
hfus	25.56	kJ/mol	Joback Method
hvap	60.52	kJ/mol	Joback Method
log10ws	-2.91		Crippen Method
logp	2.305		Crippen Method
mcvol	175.360	ml/mol	McGowan Method
pc	2354.20	kPa	Joback Method
rinpol	1895.00		NIST Webbook
tb	631.50	K	Joback Method
tc	832.05	K	Joback Method
tf	397.67	K	Joback Method
vc	0.670	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	444.17	J/molxK	631.50	Joback Method
cpg	457.90	J/molxK	664.93	Joback Method
cpg	471.00	J/molxK	698.35	Joback Method
cpg	483.43	J/molxK	731.78	Joback Method
cpg	495.19	J/molxK	765.20	Joback Method
cpg	506.25	J/molxK	798.63	Joback Method
cpg	516.59	J/molxK	832.05	Joback Method
dvisc	0.0007127	Paxs	397.67	Joback Method
dvisc	0.0004675	Paxs	436.64	Joback Method

dvisc	0.0003286	Paxs	475.61	Joback Method
dvisc	0.0002436	Paxs	514.59	Joback Method
dvisc	0.0001884	Paxs	553.56	Joback Method
dvisc	0.0001507	Paxs	592.53	Joback Method
dvisc	0.0001239	Paxs	631.50	Joback Method

Sources

Joback Method:	https://en.wikipedia.org/wiki/Joback_method
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U123085&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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
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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