

4-Dimethylamino-2-methoxybenzaldehyde

Inchi:	InChI=1S/C10H13NO2/c1-11(2)9-5-4-8(7-12)10(6-9)13-3/h4-7H,1-3H3
InchiKey:	HGDRXADJVGVGBC-UHFFFAOYSA-N
Formula:	C10H13NO2
SMILES:	COc1cc(N(C)C)ccc1C=O
Mol. weight [g/mol]:	179.22
CAS:	84562-48-1

Physical Properties

Property code	Value	Unit	Source
gf	32.73	kJ/mol	Joback Method
hf	-186.41	kJ/mol	Joback Method
hfus	21.42	kJ/mol	Joback Method
hvap	52.63	kJ/mol	Joback Method
log10ws	-1.74		Crippen Method
logp	1.574		Crippen Method
mcvol	145.420	ml/mol	McGowan Method
pc	3012.33	kPa	Joback Method
tb	548.36	K	Joback Method
tc	755.17	K	Joback Method
tf	350.62	K	Joback Method
vc	0.540	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	335.23	J/molxK	548.36	Joback Method
cpg	348.56	J/molxK	582.83	Joback Method
cpg	361.17	J/molxK	617.30	Joback Method
cpg	373.09	J/molxK	651.76	Joback Method
cpg	384.32	J/molxK	686.23	Joback Method
cpg	394.89	J/molxK	720.70	Joback Method
cpg	404.81	J/molxK	755.17	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=C84562481&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
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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