4-Dimethylamino-o-tolualdehyde

Other names: Benzaldehyde, 4-(dimethylamino)-2-methyl-
Inchi: InChI=1S/C10H13NO/c1-8-6-10(11(2)3)5-4-9(8)7-12/h4-7H,1-3H3
InchiKey: XZWMCPUAUNHGPF-UHFFFAOYSA-N
Formula: C10H13NO
SMILES: Cc1cc(N(C)C)ccc1C=O
Mol. weight [g/mol]: 163.22
CAS: 1199-59-3

Physical Properties

Property code	Value	Unit	Source
gf	137.73	kJ/mol	Joback Method
hf	-54.19	kJ/mol	Joback Method
hfus	20.23	kJ/mol	Joback Method
hvap	50.22	kJ/mol	Joback Method
log10ws	-2.10		Crippen Method
logp	1.874		Crippen Method
mcvol	139.550	ml/mol	McGowan Method
pc	3069.34	kPa	Joback Method
tb	525.94	K	Joback Method
tc	734.81	K	Joback Method
tf	328.39	K	Joback Method
vc	0.522	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	311.18	J/mol×K	525.94	Joback Method
cpg	324.80	J/mol×K	560.75	Joback Method
cpg	337.64	J/mol×K	595.56	Joback Method
cpg	349.73	J/mol×K	630.38	Joback Method
cpg	361.10	J/mol×K	665.19	Joback Method
cpg	371.77	J/mol×K	700.00	Joback Method
cpg	381.78	J/mol×K	734.81	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C1199593&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Joback Method:	https://en.wikipedia.org/wiki/Joback_method

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