

2-Propenal, 3-[4-(dimethylamino)phenyl]-

Other names:	4-Dimethylaminocinnamaldehyde 4-(N,N-Dimethylamino)cinnamaldehyde p-Dimethylaminocinnamaldehyde p-N,N-Dimethylaminocinnamaldehyde 4-Dimethylaminocinnamic aldehyde p-Dimethylaminocinnamic aldehyde Cinnamaldehyde, p-(dimethylamino)- 4-Dimethylcinnamaldehyde 3-[4-(Dimethylamino)phenyl]-2-propenal NSC 62138
Inchi:	InChI=1S/C11H13NO/c1-12(2)11-7-5-10(6-8-11)4-3-9-13/h3-9H,1-2H3/b4-3+
InchiKey:	RUKJCCIJLIMGEP-ONEGZZNKSA-N
Formula:	C11H13NO
SMILES:	CN(C)c1ccc(C=CC=O)cc1
Mol. weight [g/mol]:	175.23
CAS:	6203-18-5

Physical Properties

Property code	Value	Unit	Source
gf	236.00	kJ/mol	Joback Method
hf	53.86	kJ/mol	Joback Method
hfus	23.41	kJ/mol	Joback Method
hvap	51.74	kJ/mol	Joback Method
log10ws	-1.90		Crippen Method
logp	1.965		Crippen Method
mcvol	149.340	ml/mol	McGowan Method
pc	2973.04	kPa	Joback Method
tb	548.00	K	Joback Method
tc	761.88	K	Joback Method
tf	322.06	K	Joback Method
vc	0.558	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	338.35	J/mol×K	548.00	Joback Method
cpg	352.61	J/mol×K	583.65	Joback Method
cpg	365.91	J/mol×K	619.29	Joback Method
cpg	378.33	J/mol×K	654.94	Joback Method
cpg	389.90	J/mol×K	690.59	Joback Method
cpg	400.70	J/mol×K	726.23	Joback Method
cpg	410.77	J/mol×K	761.88	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=C6203185&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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