

4-Dimethylaminobenzoin

Other names:	Ethanone, 1-[4-(dimethylamino)phenyl]-2-hydroxy-2-phenyl- 1-Ethanone, 2-hydroxy, 1-(4-dimethylaminophenyl)-2-phenyl 1-[4-(dimethylamino)phenyl]-2-hydroxy-2-phenylethan-1-one
Inchi:	InChI=1S/C16H17NO2/c1-17(2)14-10-8-13(9-11-14)16(19)15(18)12-6-4-3-5-7-12/h3-11,
InchiKey:	SOLBSNQBVLAREX-UHFFFAOYSA-N
Formula:	C16H17NO2
SMILES:	CN(C)c1ccc(C(=O)C(O)c2ccccc2)cc1
Mol. weight [g/mol]:	255.31
CAS:	6317-85-7

Physical Properties

Property code	Value	Unit	Source
gf	141.63	kJ/mol	Joback Method
hf	-114.54	kJ/mol	Joback Method
hfus	30.07	kJ/mol	Joback Method
hvap	81.50	kJ/mol	Joback Method
log10ws	-3.38		Crippen Method
logp	2.669		Crippen Method
mcvol	206.200	ml/mol	McGowan Method
pc	2640.67	kPa	Joback Method
rinpol	2410.00		NIST Webbook
tb	781.87	K	Joback Method
tc	1002.57	K	Joback Method
tf	463.66	K	Joback Method
vc	0.752	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	586.31	J/molxK	781.87	Joback Method
cpg	599.46	J/molxK	818.65	Joback Method
cpg	611.61	J/molxK	855.44	Joback Method
cpg	622.81	J/molxK	892.22	Joback Method
cpg	633.16	J/molxK	929.00	Joback Method

cpg	642.71	J/mol×K	965.79	Joback Method
cpg	651.55	J/mol×K	1002.57	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C6317857&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
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
rinpola:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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