DIMETHYLPROPION

Other names:	1-Propanone, 2-(dimethylamino)-1-phenyl- 2-(Dimethylamino)propiophenone Dimethylpropion MG 559 Metamfepyramon Metamfepyramone NSC 234706 Propiophenone, 2-(dimethylamino)- «alpha»-Dimethylaminopropiophenone
Inchi:	InChI=1S/C11H15NO/c1-9(12(2)3)11(13)10-7-5-4-6-8-10/h4-9H,1-3H3
InchiKey:	KBHMHROOFHVLBA-UHFFFAOYSA-N
Formula:	C11H15NO
SMILES:	CC(C(=O)c1ccccc1)N(C)C
Mol. weight [g/mol]:	177.25

Physical Properties

Property code	Value	Unit	Source
af	0.4389		Cheméo Relay (1.0)
gf	133.57	kJ/mol	Joback Method
hf	-72.06	kJ/mol	Cheméo Relay (1.0)
hfus	19.38	kJ/mol	Joback Method
hvap	66.02	kJ/mol	Cheméo Relay (1.0)
ie	8.01	eV	Cheméo Relay (1.0)
log10ws	-1.07		Cheméo Relay (1.0)
logp	1.819		Crippen Method
mcvol	153.640	ml/mol	McGowan Method
pc	2847.48	kPa	Joback Method
tb	519.21	K	Cheméo Relay (1.0)
tc	730.56	K	Cheméo Relay (1.0)
tf	338.58	K	Cheméo Relay (1.0)
vc	0.550	m3/kmol	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	356.68	J/mol×K	543.63	Joback Method
cpg	372.53	J/mol×K	579.13	Joback Method
cpg	387.36	J/mol×K	614.64	Joback Method
cpg	401.22	J/mol×K	650.14	Joback Method
cpg	414.16	J/mol×K	685.65	Joback Method
cpg	426.23	J/mol×K	721.15	Joback Method
cpg	437.47	J/mol×K	756.66	Joback Method

Sources

Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws
Cheméo Relay (1.0):
Cheméo Relay (1.0, beta):
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C15351094&Units=SI
Joback Method: https://en.wikipedia.org/wiki/Joback_method
McGowan Method: http://link.springer.com/article/10.1007/BF02311772

Legend

af: Acentric Factor
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
ie: Ionization energy
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