Acetophenone, 2-phenyl-2-(4-methylphenylamino)

Inchi: InChI=1S/C21H19NO/c1-16-12-14-19(15-13-16)22-20(17-8-4-2-5-9-17)21(23)18-10-6-3-
InchiKey: OKDKHOBYMXHNMN-UHFFFAOYSA-N
Formula: C21H19NO
SMILES: Cc1ccc(NC(C(=O)c2ccccc2)c2ccccc2)cc1
Mol. weight [g/mol]: 301.38

Physical Properties

Property code	Value	Unit	Source
gf	411.57	kJ/mol	Joback Method
hf	156.96	kJ/mol	Joback Method
hfus	35.05	kJ/mol	Joback Method
hvap	82.62	kJ/mol	Joback Method
log10ws	-5.92		Crippen Method
logp	5.031		Crippen Method
mcvol	247.020	ml/mol	McGowan Method
pc	2119.73	kPa	Joback Method
rinpol	2544.00		NIST Webbook
rinpol	2544.00		NIST Webbook
tb	868.50	K	Joback Method
tc	1125.51	K	Joback Method
tf	505.80	K	Joback Method
vc	0.922	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	728.61	J/mol×K	868.50	Joback Method
cpg	743.68	J/mol×K	911.34	Joback Method
cpg	757.35	J/mol×K	954.17	Joback Method
cpg	769.75	J/mol×K	997.01	Joback Method
cpg	781.02	J/mol×K	1039.84	Joback Method
cpg	791.30	J/mol×K	1082.68	Joback Method
cpg	800.74	J/mol×K	1125.51	Joback Method

Sources

Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
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=R121123&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume