Acetoacetyldiphenylamine

Inchi: InChI=1S/C16H15NO2/c1-13(18)12-16(19)17(14-8-4-2-5-9-14)15-10-6-3-7-11-15/h2-11H
InchiKey: VLPXGVNKPRHLGC-UHFFFAOYSA-N
Formula: C16H15NO2
SMILES: CC(=O)CC(=O)N(c1ccccc1)c1ccccc1
Mol. weight [g/mol]: 253.30
CAS: 2540-31-0

Physical Properties

Property code	Value	Unit	Source
chs	-8211.90 ± 8.40	kJ/mol	NIST Webbook
gf	161.60	kJ/mol	Joback Method
hf	-58.14	kJ/mol	Joback Method
hfs	-227.90 ± 8.40	kJ/mol	NIST Webbook
hfus	31.50	kJ/mol	Joback Method
hvap	71.30	kJ/mol	Joback Method
log10ws	-3.49		Crippen Method
logp	3.330		Crippen Method
mcvol	201.900	ml/mol	McGowan Method
pc	2581.96	kPa	Joback Method
tb	739.02	K	Joback Method
tc	977.16	K	Joback Method
tf	455.25	K	Joback Method
vc	0.746	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	547.45	J/mol×K	739.02	Joback Method
cpg	562.18	J/mol×K	778.71	Joback Method
cpg	575.66	J/mol×K	818.40	Joback Method
cpg	587.96	J/mol×K	858.09	Joback Method
cpg	599.19	J/mol×K	897.78	Joback Method
cpg	609.43	J/mol×K	937.47	Joback Method
cpg	618.79	J/mol×K	977.16	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C2540310&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
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

Legend

chs:	Standard solid enthalpy of combustion
cpg:	Ideal gas heat capacity
gf:	Standard Gibbs free energy of formation
hf:	Enthalpy of formation at standard conditions
hfs:	Solid phase 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