Acrylophenone, 3,3-diphenyl-

Other names: Chalcone, «beta»-phenyl-
2-Propen-1-one, 1,3,3-triphenyl-
Inchi: InChI=1S/C21H16O/c22-21(19-14-8-3-9-15-19)16-20(17-10-4-1-5-11-17)18-12-6-2-7-13-
InchiKey: PTKAYCBILQSQRK-UHFFFAOYSA-N
Formula: C21H16O
SMILES: O=C(C=C(c1ccccc1)c1ccccc1)c1ccccc1
Mol. weight [g/mol]: 284.35
CAS: 849-01-4

Physical Properties

Property code	Value	Unit	Source
chs	-10640.00	kJ/mol	NIST Webbook
gf	405.92	kJ/mol	Joback Method
hf	227.67	kJ/mol	Joback Method
hfs	81.38	kJ/mol	NIST Webbook
hfus	32.76	kJ/mol	Joback Method
hvap	75.95	kJ/mol	Joback Method
log10ws	-5.90		Crippen Method
logp	5.001		Crippen Method
mcvol	232.740	ml/mol	McGowan Method
pc	2222.89	kPa	Joback Method
tb	817.83	K	Joback Method
tc	1087.12	K	Joback Method
tf	436.58	K	Joback Method
vc	0.875	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	648.57	J/mol×K	817.83	Joback Method
cpg	664.57	J/mol×K	862.71	Joback Method
cpg	679.12	J/mol×K	907.59	Joback Method
cpg	692.41	J/mol×K	952.48	Joback Method
cpg	704.64	J/mol×K	997.36	Joback Method

cpg	716.00	J/mol×K	1042.24	Joback Method
cpg	726.67	J/mol×K	1087.12	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C849014&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

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