3-Nitrochalcone

Other names: 2-Propen-1-one, 3-(3-nitrophenyl)-1-phenyl-
M-nitrobenzylidene acetophenone
Inchi: InChI=1S/C15H11NO3/c17-15(13-6-2-1-3-7-13)10-9-12-5-4-8-14(11-12)16(18)19/h1-11H
InchiKey: SMFBODMWKWBFOK-MDZDMXLPSA-N
Formula: C15H11NO3
SMILES: O=C(C=Cc1cccc([N+](=O)[O-])c1)c1ccccc1
Mol. weight [g/mol]: 253.25
CAS: 614-48-2

Physical Properties

Property code	Value	Unit	Source
gf	277.46	kJ/mol	Joback Method
hf	102.54	kJ/mol	Joback Method
hfus	35.46	kJ/mol	Joback Method
hvap	77.49	kJ/mol	Joback Method
log10ws	-4.84		Crippen Method
logp	3.491		Crippen Method
mcvol	189.380	ml/mol	McGowan Method
pc	2817.33	kPa	Joback Method
tb	810.81	K	Joback Method
tc	1080.95	K	Joback Method
tf	512.63	K	Joback Method
vc	0.728	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	512.78	J/mol×K	810.81	Joback Method
cpg	525.18	J/mol×K	855.83	Joback Method
cpg	536.42	J/mol×K	900.86	Joback Method
cpg	546.64	J/mol×K	945.88	Joback Method
cpg	555.98	J/mol×K	990.91	Joback Method
cpg	564.58	J/mol×K	1035.93	Joback Method
cpg	572.57	J/mol×K	1080.95	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C614482&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

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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume