p-Nitrophenacyl bromide

Other names:	4-Nitrophenacyl bromide 2-Bromo-4'-nitroacetophenone «alpha»-Bromo-p-nitroacetophenone Ethanone, 2-bromo-1-(4-nitrophenyl)- «alpha»-Bromo-4-nitroacetophenone «omega»-Bromo-p-nitroacetophenone p-Nitro-«alpha»-bromoacetophenone Acetophenone, 2-bromo-4'-nitro- Acetophenone, 2'-bromo-p-nitro- 2-Bromo-p-nitroacetophenone 2-Bromo-1-(4-nitrophenyl)ethanone 4'-Nitro-2-bromoacetophenone NSC 9805 «omega»-Bromo-4-nitroacetophenone
Inchi:	InChI=1S/C8H6BrNO3/c9-5-8(11)6-1-3-7(4-2-6)10(12)13/h1-4H,5H2
InchiKey:	MBUPVGIGAMCMBT-UHFFFAOYSA-N
Formula:	C8H6BrNO3
SMILES:	O=C(CBr)c1ccc([N+](=O)[O-])cc1
Mol. weight [g/mol]:	244.04
CAS:	99-81-0

Physical Properties

Property code	Value	Unit	Source
gf	40.21	kJ/mol	Joback Method
hf	-80.40	kJ/mol	Joback Method
hfus	28.37	kJ/mol	Joback Method
hvap	66.11	kJ/mol	Joback Method
ie	9.50	eV	NIST Webbook
ie	10.10	eV	NIST Webbook
log10ws	-3.21		Crippen Method
logp	2.172		Crippen Method
mcvol	136.310	ml/mol	McGowan Method
pc	4294.29	kPa	Joback Method
tb	685.97	K	Joback Method
tc	949.53	K	Joback Method
tf	472.20	K	Joback Method
vc	0.525	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	304.59	J/mol×K	685.97	Joback Method
cpg	313.91	J/mol×K	729.90	Joback Method
cpg	322.38	J/mol×K	773.82	Joback Method
cpg	330.05	J/mol×K	817.75	Joback Method
cpg	336.99	J/mol×K	861.67	Joback Method
cpg	343.26	J/mol×K	905.60	Joback Method
cpg	348.94	J/mol×K	949.53	Joback Method

Sources

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
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C99810&Units=SI

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
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