

2-Bromo-3'-nitroacetophenone

Other names:	«alpha»-Bromo-3-nitroacetophenone m-Nitrophenacyl bromide 3-Nitrophenacyl bromide Ethanone, 2-bromo-1-(3-nitrophenyl)- «alpha»-Bromo-m-nitroacetophenone «omega»-Bromo-m-nitroacetophenone Acetophenone, 2-bromo-3'-nitro- 2-Bromo-1-(3-nitrophenyl)ethanone 2-Bromo-1-(3-nitrophenyl)ethan-1-one
Inchi:	InChI=1S/C8H6BrNO3/c9-5-8(11)6-2-1-3-7(4-6)10(12)13/h1-4H,5H2
InchiKey:	GZHPNIQBPGUSSX-UHFFFAOYSA-N
Formula:	C8H6BrNO3
SMILES:	O=C(CBr)c1cccc([N+](=O)[O-])c1
Mol. weight [g/mol]:	244.04
CAS:	2227-64-7

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
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
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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:	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=C2227647&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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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