4-Nitrobenzoyl urea

Inchi: InChI=1S/C8H7N3O4/c9-8(13)10-7(12)5-1-3-6(4-2-5)11(14)15/h1-4H,(H3,9,10,12,13)
InchiKey: CWHBLZNYVYKDRR-UHFFFAOYSA-N
Formula: C8H7N3O4
SMILES: NC(=O)NC(=O)c1ccc([N+](=O)[O-])cc1
Mol. weight [g/mol]: 209.16
CAS: 51884-03-8

Physical Properties

Property code	Value	Unit	Source
gf	52.81	kJ/mol	Joback Method
hf	-132.05	kJ/mol	Joback Method
hfus	34.98	kJ/mol	Joback Method
hvap	83.50	kJ/mol	Joback Method
log10ws	-2.65		Crippen Method
logp	0.403		Crippen Method
mcvol	140.340	ml/mol	McGowan Method
pc	4678.49	kPa	Joback Method
tb	796.38	K	Joback Method
tc	1054.11	K	Joback Method
tf	598.25	K	Joback Method
vc	0.533	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	375.99	J/mol×K	796.38	Joback Method
cpg	384.21	J/mol×K	839.33	Joback Method
cpg	391.55	J/mol×K	882.29	Joback Method
cpg	398.08	J/mol×K	925.24	Joback Method
cpg	403.83	J/mol×K	968.20	Joback Method
cpg	408.86	J/mol×K	1011.15	Joback Method
cpg	413.22	J/mol×K	1054.11	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C51884038&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