1-(P-nitro benzoyl) semicarbazide

Inchi: InChI=1S/C8H8N4O4/c9-8(14)11-10-7(13)5-1-3-6(4-2-5)12(15)16/h1-4H,(H,10,13)(H3,9,
InchiKey: PKZCWOZBUIFLBT-UHFFFAOYSA-N
Formula: C8H8N4O4
SMILES: NC(=O)NNC(=O)c1ccc([N+](=O)[O-])cc1
Mol. weight [g/mol]: 224.17
CAS: 73859-73-1

Physical Properties

Property code	Value	Unit	Source
gf	142.20	kJ/mol	Joback Method
hf	-78.58	kJ/mol	Joback Method
hfus	40.08	kJ/mol	Joback Method
hvap	89.94	kJ/mol	Joback Method
log10ws	-2.83		Crippen Method
logp	-0.092		Crippen Method
mcvol	150.320	ml/mol	McGowan Method
pc	4762.81	kPa	Joback Method
tb	846.55	K	Joback Method
tc	1100.50	K	Joback Method
tf	650.91	K	Joback Method
vc	0.569	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	420.34	J/mol×K	846.55	Joback Method
cpg	428.10	J/mol×K	888.88	Joback Method
cpg	435.00	J/mol×K	931.20	Joback Method
cpg	441.09	J/mol×K	973.53	Joback Method
cpg	446.42	J/mol×K	1015.85	Joback Method
cpg	451.05	J/mol×K	1058.18	Joback Method
cpg	455.02	J/mol×K	1100.50	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C73859731&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

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