Benzamide, N-tetrahydrofurfuryl-4-nitro-

Inchi: InChI=1S/C12H14N2O4/c15-12(13-8-11-2-1-7-18-11)9-3-5-10(6-4-9)14(16)17/h3-6,11H,
InchiKey: ZIDAIXFZQZFHDE-UHFFFAOYSA-N
Formula: C12H14N2O4
SMILES: O=C(NCC1CCCO1)c1ccc([N+](=O)[O-])cc1
Mol. weight [g/mol]: 250.25

Physical Properties

Property code	Value	Unit	Source
gf	99.39	kJ/mol	Joback Method
hf	-207.34	kJ/mol	Joback Method
hfus	40.46	kJ/mol	Joback Method
hvap	79.78	kJ/mol	Joback Method
log10ws	-3.24		Crippen Method
logp	1.504		Crippen Method
mcvol	180.160	ml/mol	McGowan Method
pc	3103.64	kPa	Joback Method
rinpol	2244.00		NIST Webbook
rinpol	2244.00		NIST Webbook
tb	803.73	K	Joback Method
tc	1057.98	K	Joback Method
tf	547.61	K	Joback Method
vc	0.684	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	540.18	J/mol×K	803.73	Joback Method
cpg	553.46	J/mol×K	846.10	Joback Method
cpg	565.49	J/mol×K	888.48	Joback Method
cpg	576.35	J/mol×K	930.85	Joback Method
cpg	586.14	J/mol×K	973.23	Joback Method
cpg	594.94	J/mol×K	1015.60	Joback Method
cpg	602.82	J/mol×K	1057.98	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=U307349&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
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume