Benzamide, N-(3-nitrophenyl)-4-ethyl-

Inchi: InChI=1S/C15H14N2O3/c1-2-11-6-8-12(9-7-11)15(18)16-13-4-3-5-14(10-13)17(19)20/h3
InchiKey: SHAHXQBIXURWFV-UHFFFAOYSA-N
Formula: C15H14N2O3
SMILES: CCc1ccc(C(=O)Nc2cccc([N+](=O)[O-])c2)cc1
Mol. weight [g/mol]: 270.28

Physical Properties

Property code	Value	Unit	Source
gf	277.00	kJ/mol	Joback Method
hf	27.32	kJ/mol	Joback Method
hfus	39.97	kJ/mol	Joback Method
hvap	84.63	kJ/mol	Joback Method
log10ws	-4.90		Crippen Method
logp	3.410		Crippen Method
mcvol	203.660	ml/mol	McGowan Method
pc	2662.52	kPa	Joback Method
rinpol	2651.00		NIST Webbook
tb	861.80	K	Joback Method
tc	1118.69	K	Joback Method
tf	582.89	K	Joback Method
vc	0.782	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	587.55	J/mol×K	861.80	Joback Method
cpg	599.53	J/mol×K	904.61	Joback Method
cpg	610.35	J/mol×K	947.43	Joback Method
cpg	620.12	J/mol×K	990.24	Joback Method
cpg	628.91	J/mol×K	1033.06	Joback Method
cpg	636.82	J/mol×K	1075.87	Joback Method
cpg	643.93	J/mol×K	1118.69	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=U307019&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
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