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

Inchi: InChI=1S/C17H18N2O3/c1-2-3-5-13-8-10-14(11-9-13)17(20)18-15-6-4-7-16(12-15)19(21
InchiKey: VGSKIXNORZMDNL-UHFFFAOYSA-N
Formula: C17H18N2O3
SMILES: CCCCc1ccc(C(=O)Nc2cccc([N+](=O)[O-])c2)cc1
Mol. weight [g/mol]: 298.34

Physical Properties

Property code	Value	Unit	Source
gf	293.84	kJ/mol	Joback Method
hf	-13.96	kJ/mol	Joback Method
hfus	45.15	kJ/mol	Joback Method
hvap	89.09	kJ/mol	Joback Method
log10ws	-5.74		Crippen Method
logp	4.190		Crippen Method
mcvol	231.840	ml/mol	McGowan Method
pc	2204.15	kPa	Joback Method
tb	907.56	K	Joback Method
tc	1155.79	K	Joback Method
tf	605.43	K	Joback Method
vc	0.894	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	699.10	J/mol×K	907.56	Joback Method
cpg	711.56	J/mol×K	948.93	Joback Method
cpg	722.88	J/mol×K	990.30	Joback Method
cpg	733.17	J/mol×K	1031.68	Joback Method
cpg	742.51	J/mol×K	1073.05	Joback Method
cpg	750.99	J/mol×K	1114.42	Joback Method
cpg	758.71	J/mol×K	1155.79	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U306996&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