Butanamide, N-(3-nitrophenyl)-

Inchi: InChI=1S/C10H12N2O3/c1-2-4-10(13)11-8-5-3-6-9(7-8)12(14)15/h3,5-7H,2,4H2,1H3,(H,
InchiKey: VXGYYWZDOBSZDA-UHFFFAOYSA-N
Formula: C10H12N2O3
SMILES: CCCC(=O)Nc1cccc([N+](=O)[O-])c1
Mol. weight [g/mol]: 208.21

Physical Properties

Property code	Value	Unit	Source
gf	132.12	kJ/mol	Joback Method
hf	-94.54	kJ/mol	Joback Method
hfus	33.37	kJ/mol	Joback Method
hvap	70.56	kJ/mol	Joback Method
log10ws	-3.16		Crippen Method
logp	2.333		Crippen Method
mcvol	156.970	ml/mol	McGowan Method
pc	3177.55	kPa	Joback Method
rinpol	1960.00		NIST Webbook
rinpol	1960.00		NIST Webbook
tb	715.74	K	Joback Method
tc	954.01	K	Joback Method
tf	487.60	K	Joback Method
vc	0.611	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	419.01	J/mol×K	715.74	Joback Method
cpg	430.98	J/mol×K	755.45	Joback Method
cpg	442.02	J/mol×K	795.16	Joback Method
cpg	452.16	J/mol×K	834.88	Joback Method
cpg	461.45	J/mol×K	874.59	Joback Method
cpg	469.95	J/mol×K	914.30	Joback Method
cpg	477.71	J/mol×K	954.01	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=U306918&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