Propanamide, 2,2-dimethyl-N-(3-nitrophenyl)-

Other names: 2,2-Dimethyl-N-(3-nitrophenyl)propanamide
Propanamide, N-(3-nitrophenyl)-2,2-dimethyl-
Inchi: InChI=1S/C11H14N2O3/c1-11(2,3)10(14)12-8-5-4-6-9(7-8)13(15)16/h4-7H,1-3H3,(H,12,
InchiKey: YYVSAQXZGZPPHQ-UHFFFAOYSA-N
Formula: C11H14N2O3
SMILES: CC(C)(C)C(=O)Nc1cccc([N+](=O)[O-])c1
Mol. weight [g/mol]: 222.24
CAS: 32597-30-1

Physical Properties

Property code	Value	Unit	Source
gf	143.38	kJ/mol	Joback Method
hf	-123.93	kJ/mol	Joback Method
hfus	28.54	kJ/mol	Joback Method
hvap	71.50	kJ/mol	Joback Method
log10ws	-3.34		Crippen Method
logp	2.579		Crippen Method
mcvol	171.060	ml/mol	McGowan Method
pc	2918.68	kPa	Joback Method
rinpol	1867.00		NIST Webbook
rinpol	1867.00		NIST Webbook
tb	735.39	K	Joback Method
tc	982.17	K	Joback Method
tf	501.29	K	Joback Method
vc	0.655	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	473.07	J/mol×K	735.39	Joback Method
cpg	485.90	J/mol×K	776.52	Joback Method
cpg	497.64	J/mol×K	817.65	Joback Method
cpg	508.38	J/mol×K	858.78	Joback Method
cpg	518.20	J/mol×K	899.91	Joback Method

cpg	527.21	J/mol×K	941.04	Joback Method
cpg	535.49	J/mol×K	982.17	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C32597301&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
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume