1-Adamantanecarboxamide, N-(3-nitrophenyl)-

Inchi: InChI=1S/C17H20N2O3/c20-16(18-14-2-1-3-15(7-14)19(21)22)17-8-11-4-12(9-17)6-13(5
InchiKey: TZDCWSSFXSVSEK-UHFFFAOYSA-N
Formula: C17H20N2O3
SMILES: O=C(Nc1cccc([N+](=O)[O-])c1)C12CC3CC(CC(C3)C1)C2
Mol. weight [g/mol]: 300.35

Physical Properties

Property code	Value	Unit	Source
gf	348.01	kJ/mol	Joback Method
hf	-31.88	kJ/mol	Joback Method
hfus	38.57	kJ/mol	Joback Method
hvap	84.60	kJ/mol	Joback Method
log10ws	-4.81		Crippen Method
logp	3.750		Crippen Method
mcvol	223.020	ml/mol	McGowan Method
pc	2453.17	kPa	Joback Method
tb	895.96	K	Joback Method
tc	1158.94	K	Joback Method
tf	636.45	K	Joback Method
vc	0.863	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	755.36	J/mol×K	895.96	Joback Method
cpg	774.81	J/mol×K	939.79	Joback Method
cpg	794.46	J/mol×K	983.62	Joback Method
cpg	814.69	J/mol×K	1027.45	Joback Method
cpg	835.87	J/mol×K	1071.28	Joback Method
cpg	858.40	J/mol×K	1115.11	Joback Method
cpg	882.64	J/mol×K	1158.94	Joback Method

Sources

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=U307471&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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