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

Inchi: InChI=1S/C18H23NO/c1-12-3-2-4-16(5-12)19-17(20)18-9-13-6-14(10-18)8-15(7-13)11-18
InchiKey: OAAYMOQVJRKBQE-UHFFFAOYSA-N
Formula: C18H23NO
SMILES: Cc1cccc(NC(=O)C23CC4CC(CC(C4)C2)C3)c1
Mol. weight [g/mol]: 269.38

Physical Properties

Property code	Value	Unit	Source
gf	320.88	kJ/mol	Joback Method
hf	-41.76	kJ/mol	Joback Method
hfus	29.80	kJ/mol	Joback Method
hvap	70.23	kJ/mol	Joback Method
log10ws	-4.63		Crippen Method
logp	4.150		Crippen Method
mcvol	219.690	ml/mol	McGowan Method
pc	2210.37	kPa	Joback Method
rinpol	2418.00		NIST Webbook
tb	767.00	K	Joback Method
tc	1009.44	K	Joback Method
tf	504.11	K	Joback Method
vc	0.837	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	696.48	J/mol×K	767.00	Joback Method
cpg	716.70	J/mol×K	807.41	Joback Method
cpg	736.12	J/mol×K	847.81	Joback Method
cpg	755.06	J/mol×K	888.22	Joback Method
cpg	773.79	J/mol×K	928.63	Joback Method
cpg	792.61	J/mol×K	969.03	Joback Method
cpg	811.83	J/mol×K	1009.44	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=U307466&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
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume