1-Adamantanecarboxamide, N-(4-fluorophenyl)-

Inchi: InChI=1S/C17H20FNO/c18-14-1-3-15(4-2-14)19-16(20)17-8-11-5-12(9-17)7-13(6-11)10-

InchiKey: TTZQRXNXZRWGHT-UHFFFAOYSA-N

Formula: C17H20FNO

SMILES: O=C(Nc1ccc(F)cc1)C12CC3CC(CC(C3)C1)C2

Mol. weight [g/mol]: 273.35

Physical Properties

Property code	Value	Unit	Source
gf	117.65	kJ/mol	Joback Method
hf	-217.23	kJ/mol	Joback Method
hfus	30.29	kJ/mol	Joback Method
hvap	67.19	kJ/mol	Joback Method
log10ws	-4.49		Crippen Method
logp	3.981		Crippen Method
mcvol	207.370	ml/mol	McGowan Method
pc	2320.31	kPa	Joback Method
rinpol	2291.00		NIST Webbook
tb	743.39	K	Joback Method
tc	980.22	K	Joback Method
tf	493.43	K	Joback Method
vc	0.798	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	647.73	J/mol×K	743.39	Joback Method
cpg	666.65	J/mol×K	782.86	Joback Method
cpg	684.71	J/mol×K	822.33	Joback Method
cpg	702.19	J/mol×K	861.81	Joback Method
cpg	719.37	J/mol×K	901.28	Joback Method
cpg	736.51	J/mol×K	940.75	Joback Method
cpg	753.89	J/mol×K	980.22	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=U307465&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

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