1-Adamantanecarboxamide, N-(2-iodo-4-methylphenyl)-

Inchi: InChI=1S/C18H22INO/c1-11-2-3-16(15(19)4-11)20-17(21)18-8-12-5-13(9-18)7-14(6-12)1

InchiKey: VEWJBCZAHONQLT-UHFFFAOYSA-N

Formula: C18H22INO

SMILES: Cc1ccc(NC(=O)C23CC4CC(CC(C4)C2)C3)c(I)c1

Mol. weight [g/mol]: 395.28

Physical Properties

Property code	Value	Unit	Source
gf	369.37	kJ/mol	Joback Method
hf	23.64	kJ/mol	Joback Method
hfus	33.82	kJ/mol	Joback Method
hvap	80.27	kJ/mol	Joback Method
log10ws	-5.78		Crippen Method
logp	4.755		Crippen Method
mcvol	245.510	ml/mol	McGowan Method
pc	2135.43	kPa	Joback Method
tb	865.12	K	Joback Method
tc	1129.66	K	Joback Method
tf	574.69	K	Joback Method
vc	0.924	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	751.50	J/mol×K	865.12	Joback Method
cpg	771.55	J/mol×K	909.21	Joback Method
cpg	791.65	J/mol×K	953.30	Joback Method
cpg	812.18	J/mol×K	997.39	Joback Method
cpg	833.54	J/mol×K	1041.48	Joback Method
cpg	856.12	J/mol×K	1085.57	Joback Method
cpg	880.30	J/mol×K	1129.66	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=U307472&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