1,2-DIMETHYL-4-(ADAMANTYL-1)BENZENE

Other names: 1-(3,4-Dimethylphenyl)adamantane
Inchi: InChI=1S/C18H24/c1-12-3-4-17(5-13(12)2)18-9-14-6-15(10-18)8-16(7-14)11-18/h3-5,14-
InchiKey: KXXQPTCMSHPHIX-UHFFFAOYSA-N
Formula: C18H24
SMILES: Cc1ccc(C23CC4CC(CC(C4)C2)C3)cc1C
Mol. weight [g/mol]: 240.39

Physical Properties

Property code	Value	Unit	Source
hfus	22.72	kJ/mol	Joback Method
logp	4.771		Crippen Method
mcvol	208.140	ml/mol	McGowan Method
rinpol	1978.00		NIST Webbook

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	613.36	J/mol×K	667.94	Joback Method
cpg	636.13	J/mol×K	708.07	Joback Method
cpg	657.54	J/mol×K	748.21	Joback Method
cpg	677.87	J/mol×K	788.34	Joback Method
cpg	697.40	J/mol×K	828.48	Joback Method
cpg	716.40	J/mol×K	868.61	Joback Method
cpg	735.15	J/mol×K	908.75	Joback Method

Sources

Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws
Cheméo Relay (1.0):
Cheméo Relay (1.0, beta):

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C62133113&Units=SI
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

Legend

cpg:	Ideal gas heat capacity
hfus:	Enthalpy of fusion at standard conditions
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
rinpol:	Non-polar retention indices