

1,3-DIMETHYL-5-(ADAMANTYL-1)BENZENE

Other names:	1-(3,5-Dimethylphenyl)adamantane
Inchi:	InChI=1S/C18H24/c1-12-3-13(2)5-17(4-12)18-9-14-6-15(10-18)8-16(7-14)11-18/h3-5,14-
InchiKey:	QVROSZXSMHWOAF-UHFFFAOYSA-N
Formula:	C18H24
SMILES:	<chem>Cc1cc(C)cc(C23CC4CC(CC(C4)C2)C3)c1</chem>
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
mcpvol	208.140	ml/mol	McGowan Method
rinpol	1934.00		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=C73861719&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

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