

p-(Adamantyl-1)toluene

Other names:	1-(4'-Methylphenyl)adamantane 1-(4-Methylphenyl)adamantane
Inchi:	InChI=1S/C17H22/c1-12-2-4-16(5-3-12)17-9-13-6-14(10-17)8-15(7-13)11-17/h2-5,13-15
InchiKey:	RFQXTZGKFOTWFL-UHFFFAOYSA-N
Formula:	C17H22
SMILES:	<chem>Cc1ccc(C23CC4CC(CC(C4)C2)C3)cc1</chem>
Mol. weight [g/mol]:	226.36
CAS:	1459-55-8

Physical Properties

Property code	Value	Unit	Source
gf	351.99	kJ/mol	Joback Method
hf	37.99	kJ/mol	Joback Method
hfus	20.52	kJ/mol	Joback Method
hvap	54.83	kJ/mol	Joback Method
log10ws	-4.73		Crippen Method
logp	4.463		Crippen Method
mcvol	194.050	ml/mol	McGowan Method
pc	2252.53	kPa	Joback Method
tb	640.08	K	Joback Method
tc	885.25	K	Joback Method
tf	390.25	K	Joback Method
vc	0.740	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	558.71	J/molxK	640.08	Joback Method
cpg	581.57	J/molxK	680.94	Joback Method
cpg	602.87	J/molxK	721.80	Joback Method
cpg	622.91	J/molxK	762.67	Joback Method
cpg	641.99	J/molxK	803.53	Joback Method
cpg	660.41	J/molxK	844.39	Joback Method
cpg	678.46	J/molxK	885.25	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C1459558&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.cheméo.com/doc/models/crippen_log10ws
Joback Method:	https://en.wikipedia.org/wiki/Joback_method

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
h vap:	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

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