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]: 240.38
CAS: 62133-11-3

Physical Properties

Property code	Value	Unit	Source
gf	350.78	kJ/mol	Joback Method
hf	5.88	kJ/mol	Joback Method
hfus	22.72	kJ/mol	Joback Method
hvap	57.71	kJ/mol	Joback Method
log10ws	-5.21		Crippen Method
logp	4.771		Crippen Method
mcvol	208.140	ml/mol	McGowan Method
pc	2032.72	kPa	Joback Method
rinpol	1978.00		NIST Webbook
tb	667.94	K	Joback Method
tc	908.75	K	Joback Method
tf	414.04	K	Joback Method
vc	0.795	m3/kmol	Joback Method

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
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=C62133113&Units=SI

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