

2-(3-methylphenyl)-adamantane

Inchi:	InChI=1S/C17H22/c1-11-3-2-4-14(5-11)17-15-7-12-6-13(9-15)10-16(17)8-12/h2-5,12-13,
InchiKey:	DAQHMRKBAUZVPJ-ABKHHGKASA-N
Formula:	C17H22
SMILES:	Cc1cccc(C2C3CC4CC(C3)CC2C4)c1
Mol. weight [g/mol]:	226.36

Physical Properties

Property code	Value	Unit	Source
gf	349.77	kJ/mol	Joback Method
hf	2.41	kJ/mol	Joback Method
hfus	27.89	kJ/mol	Joback Method
hvap	55.67	kJ/mol	Joback Method
log10ws	-4.78		Crippen Method
logp	4.535		Crippen Method
mcvol	194.050	ml/mol	McGowan Method
pc	2094.58	kPa	Joback Method
rinpol	1875.00		NIST Webbook
tb	635.17	K	Joback Method
tc	871.06	K	Joback Method
tf	362.11	K	Joback Method
vc	0.741	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	563.17	J/molxK	635.17	Joback Method
cpg	586.65	J/molxK	674.49	Joback Method
cpg	608.42	J/molxK	713.80	Joback Method
cpg	628.63	J/molxK	753.12	Joback Method
cpg	647.42	J/molxK	792.43	Joback Method
cpg	664.95	J/molxK	831.75	Joback Method
cpg	681.35	J/molxK	871.06	Joback Method
dvisc	0.0023775	Paxs	362.11	Joback Method
dvisc	0.0023312	Paxs	407.62	Joback Method

dvisc	0.0022949	Paxs	453.13	Joback Method
dvisc	0.0022656	Paxs	498.64	Joback Method
dvisc	0.0022415	Paxs	544.15	Joback Method
dvisc	0.0022213	Paxs	589.66	Joback Method
dvisc	0.0022041	Paxs	635.17	Joback Method

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
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=R202207&Units=SI

Legend

cpg:	Ideal gas heat capacity
dvisc:	Dynamic viscosity
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

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