2-(2-methylphenyl)-adamantane

Inchi: InChI=1S/C17H22/c1-11-4-2-3-5-16(11)17-14-7-12-6-13(9-14)10-15(17)8-12/h2-5,12-15,
InchiKey: VZOUAVQIZLTWJM-DSFJPSOSSA-N
Formula: C17H22
SMILES: Cc1ccccc1C1C2CC3CC(C2)CC1C3
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	1881.00		NIST Webbook
rinpol	1881.00		NIST Webbook
tb	635.17	K	Joback Method
tc	871.06	K	Joback Method
tf	362.11	K	Joback Method
vc	0.741	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	563.17	J/mol×K	635.17	Joback Method
cpg	664.95	J/mol×K	831.75	Joback Method
cpg	647.42	J/mol×K	792.43	Joback Method
cpg	628.63	J/mol×K	753.12	Joback Method
cpg	608.42	J/mol×K	713.80	Joback Method
cpg	586.65	J/mol×K	674.49	Joback Method
cpg	681.35	J/mol×K	871.06	Joback Method
dvisc	0.0022041	Pa×s	635.17	Joback Method

dvisc	0.0022213	Pa×s	589.66	Joback Method
dvisc	0.0022415	Pa×s	544.15	Joback Method
dvisc	0.0022656	Pa×s	498.64	Joback Method
dvisc	0.0022949	Pa×s	453.13	Joback Method
dvisc	0.0023312	Pa×s	407.62	Joback Method
dvisc	0.0023775	Pa×s	362.11	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R202178&Units=SI
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

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