1-(3-methylphenyl)-adamantane

Inchi: InChI=1S/C17H22/c1-12-3-2-4-16(5-12)17-9-13-6-14(10-17)8-15(7-13)11-17/h2-5,13-15H
InchiKey: DEDRRRFOMKBUOO-QERPGXGDSA-N
Formula: C17H22
SMILES: Cc1cccc(C23CC4CC(CC(C4)C2)C3)c1
Mol. weight [g/mol]: 226.36

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
rinpol	1854.00		NIST Webbook
rinpol	1854.00		NIST Webbook
tb	640.08	K	Joback Method
tc	885.25	K	Joback Method
tf	390.25	K	Joback Method
vc	0.740	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	558.71	J/mol×K	640.08	Joback Method
cpg	581.57	J/mol×K	680.94	Joback Method
cpg	602.87	J/mol×K	721.80	Joback Method
cpg	622.91	J/mol×K	762.67	Joback Method
cpg	641.99	J/mol×K	803.53	Joback Method
cpg	660.41	J/mol×K	844.39	Joback Method
cpg	678.46	J/mol×K	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=R202138&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

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