2-(2,5-Dimethylphenyl)adamantane

Inchi: InChI=1S/C18H24/c1-11-3-4-12(2)17(5-11)18-15-7-13-6-14(9-15)10-16(18)8-13/h3-5,13-
InchiKey: CYLQZCQBTSPTOC-YREXVJSPSA-N
Formula: C18H24
SMILES: Cc1ccc(C)c(C2C3CC4CC(C3)CC2C4)c1
Mol. weight [g/mol]: 240.38

Physical Properties

Property code	Value	Unit	Source
gf	348.56	kJ/mol	Joback Method
hf	-29.70	kJ/mol	Joback Method
hfus	30.09	kJ/mol	Joback Method
hvap	58.55	kJ/mol	Joback Method
log10ws	-5.26		Crippen Method
logp	4.843		Crippen Method
mcvol	208.140	ml/mol	McGowan Method
pc	1896.95	kPa	Joback Method
rinpol	1949.00		NIST Webbook
rinpol	1949.00		NIST Webbook
tb	663.03	K	Joback Method
tc	895.09	K	Joback Method
tf	385.90	K	Joback Method
vc	0.796	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	618.70	J/mol×K	663.03	Joback Method
cpg	720.28	J/mol×K	856.41	Joback Method
cpg	702.62	J/mol×K	817.74	Joback Method
cpg	683.76	J/mol×K	779.06	Joback Method
cpg	663.58	J/mol×K	740.38	Joback Method
cpg	641.94	J/mol×K	701.71	Joback Method
cpg	736.88	J/mol×K	895.09	Joback Method
dvisc	0.0022388	Pa×s	663.03	Joback Method

dvisc	0.0022659	Pa×s	616.84	Joback Method
dvisc	0.0022979	Pa×s	570.65	Joback Method
dvisc	0.0023360	Pa×s	524.46	Joback Method
dvisc	0.0023824	Pa×s	478.28	Joback Method
dvisc	0.0024398	Pa×s	432.09	Joback Method
dvisc	0.0025130	Pa×s	385.90	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R202163&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