

2-(2,3-Dimethylphenyl)adamantane

Inchi:	InChI=1S/C18H24/c1-11-4-3-5-17(12(11)2)18-15-7-13-6-14(9-15)10-16(18)8-13/h3-5,13
InchiKey:	OUOVNLTWOACEAL-WYHCGVNCSA-N
Formula:	C18H24
SMILES:	Cc1cccc(C2C3CC4CC(C3)CC2C4)c1C
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	2006.00		NIST Webbook
rinpol	2006.00		NIST Webbook
tb	663.03	K	Joback Method
tc	895.09	K	Joback Method
tf	385.90	K	Joback Method
vc	0.796	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	618.70	J/mol×K	663.03	Joback Method
cpg	641.94	J/mol×K	701.71	Joback Method
cpg	663.58	J/mol×K	740.38	Joback Method
cpg	683.76	J/mol×K	779.06	Joback Method
cpg	702.62	J/mol×K	817.74	Joback Method
cpg	720.28	J/mol×K	856.41	Joback Method
cpg	736.88	J/mol×K	895.09	Joback Method
dvisc	0.0025130	Paxs	385.90	Joback Method

dvisc	0.0024398	Paxs	432.09	Joback Method
dvisc	0.0023824	Paxs	478.28	Joback Method
dvisc	0.0023360	Paxs	524.46	Joback Method
dvisc	0.0022979	Paxs	570.65	Joback Method
dvisc	0.0022659	Paxs	616.84	Joback Method
dvisc	0.0022388	Paxs	663.03	Joback Method

Sources

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=R202143&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071

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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