

3,5-dimethyladamantane-1-carboxylic acid, methyl ester

Inchi: InChI=1S/C14H22O2/c1-12-4-10-5-13(2,7-12)9-14(6-10,8-12)11(15)16-3/h10H,4-9H2,1-3H3
InchiKey: KKHBYYBTKDEXEI-UHFFFAOYSA-N
Formula: C14H22O2
SMILES: COC(=O)C12CC3CC(C)(CC(C)(C3)C1)C2
Mol. weight [g/mol]: 222.32

Physical Properties

Property code	Value	Unit	Source
gf	-20.95	kJ/mol	Joback Method
hf	-339.47	kJ/mol	Joback Method
hfus	9.28	kJ/mol	Joback Method
hvap	52.06	kJ/mol	Joback Method
log10ws	-3.26		Crippen Method
logp	3.156		Crippen Method
mcvol	182.980	ml/mol	McGowan Method
pc	2502.50	kPa	Joback Method
rinpol	1467.00		NIST Webbook
rinpol	1490.00		NIST Webbook
rinpol	1482.00		NIST Webbook
rinpol	1467.00		NIST Webbook
rinpol	1501.00		NIST Webbook
ripol	1888.00		NIST Webbook
ripol	1850.00		NIST Webbook
ripol	1869.00		NIST Webbook
tb	616.55	K	Joback Method
tc	848.72	K	Joback Method
tf	437.46	K	Joback Method
vc	0.700	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	522.30	J/mol×K	616.55	Joback Method
cpg	541.87	J/mol×K	655.25	Joback Method

cpg	560.38	J/mol×K	693.94	Joback Method
cpg	578.24	J/mol×K	732.64	Joback Method
cpg	595.89	J/mol×K	771.33	Joback Method
cpg	613.76	J/mol×K	810.03	Joback Method
cpg	632.26	J/mol×K	848.72	Joback Method

Sources

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=R304680&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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
ripol:	Polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

Latest version available from:

<https://www.chemeo.com/cid/13-173-5/3-5-dimethyladamantane-1-carboxylic-acid-methyl-ester.pdf>

Generated by Cheméo on 2025-12-05 09:23:53.770819846 +0000 UTC m=+4674831.300860499.

Cheméo (<https://www.chemeo.com>) is the biggest free database of chemical and physical data for the process industry.