

3-ethyladamantane-1-carboxylic acid, methyl ester

Inchi:	InChI=1S/C14H22O2/c1-3-13-5-10-4-11(6-13)8-14(7-10,9-13)12(15)16-2/h10-11H,3-9H2
InchiKey:	ZWAHRPCXTAHOBO-UHFFFAOYSA-N
Formula:	C14H22O2
SMILES:	CCC12CC3CC(C1)CC(C(=O)OC)(C3)C2
Mol. weight [g/mol]:	222.32

Physical Properties

Property code	Value	Unit	Source
gf	-15.46	kJ/mol	Joback Method
hf	-354.71	kJ/mol	Joback Method
hfus	15.58	kJ/mol	Joback Method
hvap	53.21	kJ/mol	Joback Method
log10ws	-3.26		Crippen Method
logp	3.156		Crippen Method
mcvol	182.980	ml/mol	McGowan Method
pc	2393.53	kPa	Joback Method
ripol	1604.00		NIST Webbook
ripol	1618.00		NIST Webbook
ripol	1579.00		NIST Webbook
ripol	1579.00		NIST Webbook
ripol	1594.00		NIST Webbook
ripol	2028.00		NIST Webbook
ripol	2051.00		NIST Webbook
ripol	2028.00		NIST Webbook
tb	616.31	K	Joback Method
tc	839.69	K	Joback Method
tf	413.56	K	Joback Method
vc	0.702	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	524.80	J/molxK	616.31	Joback Method
cpg	544.54	J/molxK	653.54	Joback Method

cpg	563.15	J/mol×K	690.77	Joback Method
cpg	580.89	J/mol×K	728.00	Joback Method
cpg	598.06	J/mol×K	765.23	Joback Method
cpg	614.94	J/mol×K	802.46	Joback Method
cpg	631.82	J/mol×K	839.69	Joback Method

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
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=R304724&Units=SI

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
rinpola:	Non-polar retention indices
ripola:	Polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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