4e-methyladamantane-1e-carboxylic acid, methyl ester

Inchi: InChI=1S/C13H20O2/c1-8-10-3-9-4-11(8)7-13(5-9,6-10)12(14)15-2/h8-11H,3-7H2,1-2H3
InchiKey: GPDUTWRPOYXFNJ-JTPDLKOHSA-N
Formula: C13H20O2
SMILES: COC(=O)C12CC3CC(C1)C(C)C(C3)C2
Mol. weight [g/mol]: 208.30

Physical Properties

Property code	Value	Unit	Source
gf	-26.10	kJ/mol	Joback Method
hf	-369.65	kJ/mol	Joback Method
hfus	20.36	kJ/mol	Joback Method
hvap	51.83	kJ/mol	Joback Method
log10ws	-2.60		Crippen Method
logp	2.622		Crippen Method
mcvol	168.890	ml/mol	McGowan Method
pc	2436.25	kPa	Joback Method
rinpol	1550.00		NIST Webbook
rinpol	1512.00		NIST Webbook
rinpol	1537.00		NIST Webbook
rinpol	1524.00		NIST Webbook
rinpol	1512.00		NIST Webbook
ripol	1951.00		NIST Webbook
ripol	1996.00		NIST Webbook
ripol	1974.00		NIST Webbook
ripol	1951.00		NIST Webbook
tb	588.52	K	Joback Method
tc	807.42	K	Joback Method
tf	374.15	K	Joback Method
vc	0.646	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	476.26	J/mol×K	588.52	Joback Method

cpg	496.38	J/mol×K	625.00	Joback Method
cpg	515.21	J/mol×K	661.49	Joback Method
cpg	532.92	J/mol×K	697.97	Joback Method
cpg	549.69	J/mol×K	734.45	Joback Method
cpg	565.68	J/mol×K	770.93	Joback Method
cpg	581.06	J/mol×K	807.42	Joback Method

Sources

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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R383896&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
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