Adamantan-1-carboxylic acid, methyl ester

Other names: Adamantane-1-carboxylic acid, methyl ester
1-Adamantanecarboxylic acid, methyl ester
Tricyclo[3.3.1.1
Inchi: InChI=1S/C12H18O2/c1-14-11(13)12-5-8-2-9(6-12)4-10(3-8)7-12/h8-10H,2-7H2,1H3
InchiKey: CLYOOVNORYNXMD-UHFFFAOYSA-N
Formula: C12H18O2
SMILES: COC(=O)C12CC3CC(CC(C3)C1)C2
Mol. weight [g/mol]: 194.27
CAS: 711-01-3

Physical Properties

Property code	Value	Unit	Source
affp	864.10	kJ/mol	NIST Webbook
basg	833.10	kJ/mol	NIST Webbook
chs	-6716.80 ± 2.10	kJ/mol	NIST Webbook
gf	-26.81	kJ/mol	Joback Method
hf	-495.40 ± 2.70	kJ/mol	NIST Webbook
hfs	-577.80 ± 2.60	kJ/mol	NIST Webbook
hfus	16.70	kJ/mol	Joback Method
hsub	82.40	kJ/mol	NIST Webbook
hsub	82.40 ± 0.60	kJ/mol	NIST Webbook
hsub	82.40 ± 0.60	kJ/mol	NIST Webbook
hvap	49.91	kJ/mol	Joback Method
ie	9.38 ± 0.03	eV	NIST Webbook
log10ws	-2.43		Crippen Method
logp	2.376		Crippen Method
mcvol	154.800	ml/mol	McGowan Method
pc	2778.85	kPa	Joback Method
rinpol	1431.00		NIST Webbook
rinpol	1489.00		NIST Webbook
rinpol	1449.00		NIST Webbook
rinpol	1465.00		NIST Webbook
rinpol	1474.00		NIST Webbook
rinpol	1486.00		NIST Webbook
rinpol	1489.00		NIST Webbook
rinpol	1486.00		NIST Webbook
ripol	1858.00		NIST Webbook

ripol	1892.00		NIST Webbook
ripol	1914.00		NIST Webbook
ripol	1937.00		NIST Webbook
ripol	1858.00		NIST Webbook
tb	570.31	K	Joback Method
tc	793.24	K	Joback Method
tf	367.12	K	Joback Method
vc	0.592	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	424.27	J/mol×K	570.31	Joback Method
cpg	443.51	J/mol×K	607.47	Joback Method
cpg	461.41	J/mol×K	644.62	Joback Method
cpg	478.15	J/mol×K	681.78	Joback Method
cpg	493.91	J/mol×K	718.93	Joback Method
cpg	508.89	J/mol×K	756.09	Joback Method
cpg	523.27	J/mol×K	793.24	Joback Method
cps	264.20	J/mol×K	298.15	NIST Webbook
hsubt	84.30 ± 0.60	kJ/mol	275.00	NIST Webbook

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C711013&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

affp: Proton affinity
basg: Gas basicity
chs: Standard solid enthalpy of combustion
cpg: Ideal gas heat capacity

cps:	Solid phase heat capacity
gf:	Standard Gibbs free energy of formation
hf:	Enthalpy of formation at standard conditions
hfs:	Solid phase enthalpy of formation at standard conditions
hfus:	Enthalpy of fusion at standard conditions
hsub:	Enthalpy of sublimation at standard conditions
hsubt:	Enthalpy of sublimation at a given temperature
hvap:	Enthalpy of vaporization at standard conditions
ie:	Ionization energy
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