4-Carbomethoxyhomocubane

Inchi: InChI=1S/C11H12O2/c1-13-10(12)11-7-4-2-3-5(7)9(11)6(3)8(4)11/h3-9H,2H2,1H3
InchiKey: VZNFAXUDGDVVBT-UHFFFAOYSA-N
Formula: C11H12O2
SMILES: COC(=O)C12C3C4CC5C3C1C5C42
Mol. weight [g/mol]: 176.21
CAS: 40317-63-3

Physical Properties

Property code	Value	Unit	Source
chl	-5989.80 ± 5.00	kJ/mol	NIST Webbook
gf	155.55	kJ/mol	Joback Method
hf	26.00 ± 5.40	kJ/mol	NIST Webbook
hfl	-54.00 ± 5.00	kJ/mol	NIST Webbook
hfus	27.22	kJ/mol	Joback Method
hvap	80.00	kJ/mol	NIST Webbook
log10ws	-0.83		Crippen Method
logp	0.917		Crippen Method
mcvol	118.990	ml/mol	McGowan Method
pc	3149.09	kPa	Joback Method
tb	521.68	K	Joback Method
tc	726.36	K	Joback Method
tf	407.89	K	Joback Method
vc	0.503	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	386.58	J/mol×K	624.02	Joback Method
cpg	398.14	J/mol×K	658.13	Joback Method
cpg	408.95	J/mol×K	692.25	Joback Method
cpg	345.11	J/mol×K	521.68	Joback Method
cpg	360.29	J/mol×K	555.79	Joback Method
cpg	374.04	J/mol×K	589.91	Joback Method
cpg	419.22	J/mol×K	726.36	Joback Method

cpl	288.00	J/mol×K	298.00	NIST Webbook
hvapt	79.96	kJ/mol	323.00	NIST Webbook
hvapt	80.00 ± 2.00	kJ/mol	303.00	NIST Webbook
hvapt	80.00 ± 1.70	kJ/mol	323.00	NIST Webbook

Sources

McGowan Method: http://link.springer.com/article/10.1007/BF02311772
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C40317633&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

Legend

chl: Standard liquid enthalpy of combustion
cpg: Ideal gas heat capacity
cpl: Liquid phase heat capacity
gf: Standard Gibbs free energy of formation
hf: Enthalpy of formation at standard conditions
hfl: Liquid phase enthalpy of formation at standard conditions
hfus: Enthalpy of fusion at standard conditions
hvap: Enthalpy of vaporization at standard conditions
hvapt: Enthalpy of vaporization at a given temperature
log10ws: Log10 of Water solubility in mol/l
logp: Octanol/Water partition coefficient
mcvol: McGowan's characteristic volume
pc: Critical Pressure
tb: Normal Boiling Point Temperature
tc: Critical Temperature
tf: Normal melting (fusion) point
vc: Critical Volume