Methyl cyclocopacamphanoate

Inchi: InChI=1S/C16H24O2/c1-8(14(17)18-4)10-6-5-9-11-7-12-13(9)16(12,3)15(10,11)2/h8-13H
InchiKey: VAUWHFXQUIWJJY-TZWADDNZSA-N
Formula: C16H24O2
SMILES: COC(=O)C(C)C1CCC2C3CC4C2C4(C)C13C
Mol. weight [g/mol]: 248.36

Physical Properties

Property code	Value	Unit	Source
gf	80.57	kJ/mol	Joback Method
hf	-350.67	kJ/mol	Joback Method
hfus	23.82	kJ/mol	Joback Method
hvap	56.06	kJ/mol	Joback Method
log10ws	-3.03		Crippen Method
logp	3.114		Crippen Method
mcvol	200.300	ml/mol	McGowan Method
pc	1994.77	kPa	Joback Method
rinpol	1614.00		NIST Webbook
rinpol	1614.00		NIST Webbook
tb	646.22	K	Joback Method
tc	859.88	K	Joback Method
tf	441.12	K	Joback Method
vc	0.786	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	614.24	J/mol×K	646.22	Joback Method
cpg	634.03	J/mol×K	681.83	Joback Method
cpg	652.86	J/mol×K	717.44	Joback Method
cpg	671.03	J/mol×K	753.05	Joback Method
cpg	688.84	J/mol×K	788.66	Joback Method
cpg	706.56	J/mol×K	824.27	Joback Method
cpg	724.51	J/mol×K	859.88	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R199181&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

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