6-Hydroxymethylbicyclo[2.2.1]hept-2-ene-1-carbo acid, methyl ester

Inchi: InChI=1S/C10H14O3/c1-13-9(12)10-3-2-7(5-10)4-8(10)6-11/h2-3,7-8,11H,4-6H2,1H3
InchiKey: MTAURAMEOVOLEM-UHFFFAOYSA-N
Formula: C10H14O3
SMILES: COC(=O)C12C=CC(CC1CO)C2
Mol. weight [g/mol]: 182.22

Physical Properties

Property code	Value	Unit	Source
gf	-211.26	kJ/mol	Joback Method
hf	-454.64	kJ/mol	Joback Method
hfus	18.70	kJ/mol	Joback Method
hvap	62.52	kJ/mol	Joback Method
log10ws	-1.05		Crippen Method
logp	0.734		Crippen Method
mcvol	139.050	ml/mol	McGowan Method
pc	3431.89	kPa	Joback Method
rinpol	1368.00		NIST Webbook
rinpol	1368.00		NIST Webbook
tb	609.15	K	Joback Method
tc	810.61	K	Joback Method
tf	388.22	K	Joback Method
vc	0.527	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	379.28	J/mol×K	609.15	Joback Method
cpg	392.05	J/mol×K	642.73	Joback Method
cpg	404.09	J/mol×K	676.30	Joback Method
cpg	415.52	J/mol×K	709.88	Joback Method
cpg	426.45	J/mol×K	743.45	Joback Method
cpg	436.99	J/mol×K	777.03	Joback Method
cpg	447.25	J/mol×K	810.61	Joback Method

Sources

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=U186817&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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