Bicyclo[2.2.1]hept-5-ene-2-carboxylic acid, methyl ester, exo-

Other names: cis-Bicyclo[2.2.1]hept-2-ene-5-carboxylic acid, methyl ester
exo-Bicyclo[2.2.1]hept-5-en-2-carboxylic acid, methyl ester
Inchi: InChI=1S/C9H12O2/c1-11-9(10)8-5-6-2-3-7(8)4-6/h2-3,6-8H,4-5H2,1H3/t6-,7-,8+/m1/s1
InchiKey: RMAZRAQKPTXZNL-PRJMDXOYSA-N
Formula: C9H12O2
SMILES: COC(=O)C1CC2C=CC1C2
Mol. weight [g/mol]: 152.19
CAS: 769-85-7

Physical Properties

Property code	Value	Unit	Source
gf	-77.37	kJ/mol	Joback Method
hf	-297.01	kJ/mol	Joback Method
hfus	18.32	kJ/mol	Joback Method
hvap	44.77	kJ/mol	Joback Method
log10ws	-1.37		Crippen Method
logp	1.372		Crippen Method
mcvol	119.090	ml/mol	McGowan Method
pc	3272.78	kPa	Joback Method
rinpol	1098.00		NIST Webbook
rinpol	1098.00		NIST Webbook
ripol	1493.00		NIST Webbook
tb	493.85	K	Joback Method
tc	704.70	K	Joback Method
tf	292.23	K	Joback Method
vc	0.455	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	278.17	J/mol×K	493.85	Joback Method
cpg	346.34	J/mol×K	669.56	Joback Method
cpg	334.41	J/mol×K	634.41	Joback Method
cpg	321.67	J/mol×K	599.27	Joback Method

cpg	308.08	J/mol×K	564.13	Joback Method
cpg	293.60	J/mol×K	528.99	Joback Method
cpg	357.51	J/mol×K	704.70	Joback Method
dvisc	0.0007920	Pa×s	493.85	Joback Method
dvisc	0.0008358	Pa×s	460.25	Joback Method
dvisc	0.0008896	Pa×s	426.64	Joback Method
dvisc	0.0009570	Pa×s	393.04	Joback Method
dvisc	0.0010436	Pa×s	359.44	Joback Method
dvisc	0.0011587	Pa×s	325.83	Joback Method
dvisc	0.0013177	Pa×s	292.23	Joback Method

Sources

McGowan Method: http://link.springer.com/article/10.1007/BF02311772
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C769857&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

cpg: Ideal gas heat capacity
dvisc: Dynamic viscosity
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