Bicyclo[2.2.1]heptane-2-carboxylic acid, methyl ester

Other names: 2-Norbornanecarboxylic acid, methyl ester
Inchi: InChI=1S/C9H14O2/c1-11-9(10)8-5-6-2-3-7(8)4-6/h6-8H,2-5H2,1H3
InchiKey: BWGIKEUGPCOETD-UHFFFAOYSA-N
Formula: C9H14O2
SMILES: COC(=O)C1CC2CCC1C2
Mol. weight [g/mol]: 154.21
CAS: 35520-81-1

Physical Properties

Property code	Value	Unit	Source
gf	-107.33	kJ/mol	Joback Method
hf	-354.79	kJ/mol	Joback Method
hfus	17.09	kJ/mol	Joback Method
hvap	44.47	kJ/mol	Joback Method
log10ws	-1.52		Crippen Method
logp	1.596		Crippen Method
mcvol	123.390	ml/mol	McGowan Method
pc	3142.03	kPa	Joback Method
rinpol	1135.00		NIST Webbook
rinpol	1135.00		NIST Webbook
ripol	1512.00		NIST Webbook
ripol	1512.00		NIST Webbook
tb	494.69	K	Joback Method
tc	703.45	K	Joback Method
tf	291.47	K	Joback Method
vc	0.469	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	294.85	J/mol×K	494.69	Joback Method
cpg	311.49	J/mol×K	529.48	Joback Method
cpg	327.15	J/mol×K	564.28	Joback Method
cpg	341.89	J/mol×K	599.07	Joback Method

cpg	355.75	J/mol×K	633.86	Joback Method
cpg	368.76	J/mol×K	668.65	Joback Method
cpg	380.99	J/mol×K	703.45	Joback Method
dvisc	0.0015354	Pa×s	291.47	Joback Method
dvisc	0.0013027	Pa×s	325.34	Joback Method
dvisc	0.0011401	Pa×s	359.21	Joback Method
dvisc	0.0010209	Pa×s	393.08	Joback Method
dvisc	0.0009304	Pa×s	426.95	Joback Method
dvisc	0.0008595	Pa×s	460.82	Joback Method
dvisc	0.0008027	Pa×s	494.69	Joback Method

Sources

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
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C35520811&Units=SI

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