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

Other names: Ethyl 5-norbornene-2-carboxylate
2,5-Endomethylene-3-cyclohexene carboxylic acid, ethyl ester
5-Norbornene-2-carboxylic acid, ethyl ester

Inchi: InChI=1S/C10H14O2/c1-2-12-10(11)9-6-7-3-4-8(9)5-7/h3-4,7-9H,2,5-6H2,1H3

InchiKey: FCCGTJAGEHZPBF-UHFFFAOYSA-N

Formula: C10H14O2

SMILES: CCOC(=O)C1CC2C=CC1C2

Mol. weight [g/mol]: 166.22

CAS: 10138-32-6

Physical Properties

Property code	Value	Unit	Source
gf	-68.95	kJ/mol	Joback Method
hf	-317.65	kJ/mol	Joback Method
hfus	20.91	kJ/mol	Joback Method
hvap	46.99	kJ/mol	Joback Method
log10ws	-1.79		Crippen Method
logp	1.762		Crippen Method
mcvol	133.180	ml/mol	McGowan Method
pc	2940.89	kPa	Joback Method
tb	516.73	K	Joback Method
tc	724.41	K	Joback Method
tf	303.50	K	Joback Method
vc	0.510	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	323.62	J/mol×K	516.73	Joback Method
cpg	395.51	J/mol×K	689.79	Joback Method
cpg	382.88	J/mol×K	655.18	Joback Method
cpg	369.42	J/mol×K	620.57	Joback Method
cpg	355.09	J/mol×K	585.96	Joback Method
cpg	339.84	J/mol×K	551.34	Joback Method

cpg	407.35	J/mol×K	724.41	Joback Method
dvisc	0.0008232	Pa×s	516.73	Joback Method
dvisc	0.0008790	Pa×s	481.19	Joback Method
dvisc	0.0009484	Pa×s	445.65	Joback Method
dvisc	0.0010369	Pa×s	410.12	Joback Method
dvisc	0.0011529	Pa×s	374.58	Joback Method
dvisc	0.0013107	Pa×s	339.04	Joback Method
dvisc	0.0015357	Pa×s	303.50	Joback Method

Sources

McGowan Method: http://link.springer.com/article/10.1007/BF02311772
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C10138326&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
tb: Normal Boiling Point Temperature
tc: Critical Temperature
tf: Normal melting (fusion) point
vc: Critical Volume