

Bicyclo[2.2.1]heptane, 2-(1-methoxyethylidene)-, (E)-

Inchi:	InChI=1S/C10H16O/c1-7(11-2)10-6-8-3-4-9(10)5-8/h8-9H,3-6H2,1-2H3/b10-7+
InchiKey:	NXHRRGXAJNAGTQ-JXMROGBWSA-N
Formula:	C10H16O
SMILES:	COC(C)=C1CC2CCC1C2
Mol. weight [g/mol]:	152.23
CAS:	103582-45-2

Physical Properties

Property code	Value	Unit	Source
gf	74.63	kJ/mol	Joback Method
hf	-176.27	kJ/mol	Joback Method
hfus	16.03	kJ/mol	Joback Method
hvap	41.13	kJ/mol	Joback Method
log10ws	-2.75		Crippen Method
logp	2.727		Crippen Method
mcvol	131.610	ml/mol	McGowan Method
pc	2841.41	kPa	Joback Method
tb	474.89	K	Joback Method
tc	681.99	K	Joback Method
tf	253.45	K	Joback Method
vc	0.503	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	299.45	J/molxK	474.89	Joback Method
cpg	316.93	J/molxK	509.41	Joback Method
cpg	333.39	J/molxK	543.92	Joback Method
cpg	348.87	J/molxK	578.44	Joback Method
cpg	363.44	J/molxK	612.96	Joback Method
cpg	377.15	J/molxK	647.47	Joback Method
cpg	390.05	J/molxK	681.99	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=C103582452&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071

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

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