Bicyclo[2.2.2]oct-2-ene-1-carboxylic acid

Inchi: InChI=1S/C9H12O2/c10-8(11)9-4-1-7(2-5-9)3-6-9/h1,4,7H,2-3,5-6H2,(H,10,11)
InchiKey: CKHVIPJAGMCQPO-UHFFFAOYSA-N
Formula: C9H12O2
SMILES: O=C(O)C12C=CC(CC1)CC2
Mol. weight [g/mol]: 152.19
CAS: 2534-80-7

Physical Properties

Property code	Value	Unit	Source
gf	-119.07	kJ/mol	Joback Method
hf	-287.60	kJ/mol	Joback Method
hfus	11.75	kJ/mol	Joback Method
hvap	58.36	kJ/mol	Joback Method
log10ws	-1.85		Crippen Method
logp	1.817		Crippen Method
mcvol	119.090	ml/mol	McGowan Method
pc	4238.55	kPa	Joback Method
tb	572.79	K	Joback Method
tc	786.54	K	Joback Method
tf	355.44	K	Joback Method
vc	0.447	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	306.53	J/mol×K	572.79	Joback Method
cpg	319.26	J/mol×K	608.41	Joback Method
cpg	331.07	J/mol×K	644.04	Joback Method
cpg	342.10	J/mol×K	679.66	Joback Method
cpg	352.50	J/mol×K	715.29	Joback Method
cpg	362.42	J/mol×K	750.91	Joback Method
cpg	371.99	J/mol×K	786.54	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C2534807&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
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

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