Bicyclo[2.2.2]octane-1-carboxylic acid

Inchi: InChI=1S/C9H14O2/c10-8(11)9-4-1-7(2-5-9)3-6-9/h7H,1-6H2,(H,10,11)
InchiKey: PUNFICOCZAPAJV-UHFFFAOYSA-N
Formula: C9H14O2
SMILES: O=C(O)C12CCC(CC1)CC2
Mol. weight [g/mol]: 154.21
CAS: 699-55-8

Physical Properties

Property code	Value	Unit	Source
gf	-149.03	kJ/mol	Joback Method
hf	-345.38	kJ/mol	Joback Method
hfus	10.53	kJ/mol	Joback Method
hvap	58.07	kJ/mol	Joback Method
log10ws	-1.99		Crippen Method
logp	2.041		Crippen Method
mcvol	123.390	ml/mol	McGowan Method
pc	4046.64	kPa	Joback Method
tb	573.63	K	Joback Method
tc	785.40	K	Joback Method
tf	354.68	K	Joback Method
vc	0.461	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	326.21	J/mol×K	573.63	Joback Method
cpg	340.09	J/mol×K	608.92	Joback Method
cpg	353.02	J/mol×K	644.22	Joback Method
cpg	365.14	J/mol×K	679.51	Joback Method
cpg	376.58	J/mol×K	714.81	Joback Method
cpg	387.49	J/mol×K	750.10	Joback Method
cpg	398.01	J/mol×K	785.40	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=C699558&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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