Bicyclo[2.2.2]octane-1-carboxylic acid, 4-methyl-

Other names: 4-Methylbicyclo[2.2.2]octane-1-carboxylic acid
Inchi: InChI=1S/C10H16O2/c1-9-2-5-10(6-3-9,7-4-9)8(11)12/h2-7H2,1H3,(H,11,12)
InchiKey: VAIOYMYTWWCODC-UHFFFAOYSA-N
Formula: C10H16O2
SMILES: CC12CCC(C(=O)O)(CC1)CC2
Mol. weight [g/mol]: 168.23
CAS: 702-67-0

Physical Properties

Property code	Value	Unit	Source
gf	-146.10	kJ/mol	Joback Method
hf	-350.78	kJ/mol	Joback Method
hfus	6.82	kJ/mol	Joback Method
hvap	59.15	kJ/mol	Joback Method
log10ws	-2.41		Crippen Method
logp	2.432		Crippen Method
mcvol	137.480	ml/mol	McGowan Method
pc	3796.32	kPa	Joback Method
tb	596.75	K	Joback Method
tc	813.10	K	Joback Method
tf	389.85	K	Joback Method
vc	0.514	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	372.23	J/mol×K	596.75	Joback Method
cpg	386.35	J/mol×K	632.81	Joback Method
cpg	399.58	J/mol×K	668.87	Joback Method
cpg	412.15	J/mol×K	704.92	Joback Method
cpg	424.30	J/mol×K	740.98	Joback Method
cpg	436.27	J/mol×K	777.04	Joback Method
cpg	448.30	J/mol×K	813.10	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C702670&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