Bicyclo[2.2.1]heptan-3-one, 1,4,7-trimethyl

Inchi: InChI=1S/C10H16O/c1-7-9(2)4-5-10(7,3)8(11)6-9/h7H,4-6H2,1-3H3
InchiKey: XWDFUXPMQMTMTC-UHFFFAOYSA-N
Formula: C10H16O
SMILES: CC1C2(C)CCC1(C)C(=O)C2
Mol. weight [g/mol]: 152.23

Physical Properties

Property code	Value	Unit	Source
gf	1.44	kJ/mol	Joback Method
hf	-237.85	kJ/mol	Joback Method
hfus	3.81	kJ/mol	Joback Method
hvap	39.49	kJ/mol	Joback Method
log10ws	-2.35		Crippen Method
logp	2.402		Crippen Method
mcvol	131.610	ml/mol	McGowan Method
pc	3082.99	kPa	Joback Method
rinpol	1126.00		NIST Webbook
rinpol	1126.00		NIST Webbook
tb	509.58	K	Joback Method
tc	742.46	K	Joback Method
tf	346.60	K	Joback Method
vc	0.503	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	324.29	J/mol×K	509.58	Joback Method
cpg	342.61	J/mol×K	548.39	Joback Method
cpg	359.48	J/mol×K	587.21	Joback Method
cpg	375.18	J/mol×K	626.02	Joback Method
cpg	389.96	J/mol×K	664.83	Joback Method
cpg	404.06	J/mol×K	703.65	Joback Method
cpg	417.76	J/mol×K	742.46	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=R324639&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
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume