4,7-Dimethylbicyclo[3.2.1]oct-3-en-6-one

Inchi: InChI=1S/C10H14O/c1-6-3-4-8-5-9(6)10(11)7(8)2/h3,7-9H,4-5H2,1-2H3
InchiKey: QTERZTSMYKWUDY-UHFFFAOYSA-N
Formula: C10H14O
SMILES: CC1=CCC2CC1C(=O)C2C
Mol. weight [g/mol]: 150.22

Physical Properties

Property code	Value	Unit	Source
gf	20.65	kJ/mol	Joback Method
hf	-228.18	kJ/mol	Joback Method
hfus	15.14	kJ/mol	Joback Method
hvap	42.92	kJ/mol	Joback Method
log10ws	-2.21		Crippen Method
logp	2.178		Crippen Method
mcvol	127.310	ml/mol	McGowan Method
pc	2937.70	kPa	Joback Method
rinpol	1180.00		NIST Webbook
tb	517.51	K	Joback Method
tc	742.98	K	Joback Method
tf	308.56	K	Joback Method
vc	0.485	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	307.68	J/mol×K	517.51	Joback Method
cpg	325.53	J/mol×K	555.09	Joback Method
cpg	342.41	J/mol×K	592.67	Joback Method
cpg	358.33	J/mol×K	630.24	Joback Method
cpg	373.32	J/mol×K	667.82	Joback Method
cpg	387.41	J/mol×K	705.40	Joback Method
cpg	400.62	J/mol×K	742.98	Joback Method

Sources

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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R589465&Units=SI

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