4,7,7-Trimethylbicyclo[3.2.0]hept-3-en-6-one

Inchi: InChI=1S/C10H14O/c1-6-4-5-7-8(6)9(11)10(7,2)3/h4,7-8H,5H2,1-3H3
InchiKey: JVEJBTZZORGEKF-UHFFFAOYSA-N
Formula: C10H14O
SMILES: CC1=CCC2C1C(=O)C2(C)C
Mol. weight [g/mol]: 150.22
CAS: 4613-37-0

Physical Properties

Property code	Value	Unit	Source
gf	27.26	kJ/mol	Joback Method
hf	-206.78	kJ/mol	Joback Method
hfus	10.94	kJ/mol	Joback Method
hvap	41.59	kJ/mol	Joback Method
log10ws	-2.21		Crippen Method
logp	2.178		Crippen Method
mcvol	127.310	ml/mol	McGowan Method
pc	3002.44	kPa	Joback Method
rinpol	1083.00		NIST Webbook
rinpol	1083.00		NIST Webbook
rinpol	1109.00		NIST Webbook
rinpol	1107.70		NIST Webbook
rinpol	1109.00		NIST Webbook
ripol	1445.00		NIST Webbook
tb	513.48	K	Joback Method
tc	740.08	K	Joback Method
tf	335.98	K	Joback Method
vc	0.491	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	307.39	J/mol×K	513.48	Joback Method
cpg	324.08	J/mol×K	551.25	Joback Method
cpg	339.67	J/mol×K	589.01	Joback Method

cpg	354.29	J/mol×K	626.78	Joback Method
cpg	368.08	J/mol×K	664.55	Joback Method
cpg	381.17	J/mol×K	702.31	Joback Method
cpg	393.70	J/mol×K	740.08	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=C4613370&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
ripol:	Polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume