3,6,6-Trimethylbicyclo-[3.1.0]-hexane-3-carboxald

Inchi: InChI=1S/C10H16O/c1-9(2)7-4-10(3,6-11)5-8(7)9/h6-8H,4-5H2,1-3H3
InchiKey: HODJJSXHJFNBQH-UHFFFAOYSA-N
Formula: C10H16O
SMILES: CC1(C=O)CC2C(C1)C2(C)C
Mol. weight [g/mol]: 152.23

Physical Properties

Property code	Value	Unit	Source
gf	28.90	kJ/mol	Joback Method
hf	-199.91	kJ/mol	Joback Method
hfus	9.76	kJ/mol	Joback Method
hvap	41.48	kJ/mol	Joback Method
log10ws	-2.11		Crippen Method
logp	2.258		Crippen Method
mcvol	131.610	ml/mol	McGowan Method
pc	3018.96	kPa	Joback Method
ripol	1547.00		NIST Webbook
tb	481.48	K	Joback Method
tc	693.12	K	Joback Method
tf	319.66	K	Joback Method
vc	0.520	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	316.35	J/mol×K	481.48	Joback Method
cpg	333.54	J/mol×K	516.75	Joback Method
cpg	349.24	J/mol×K	552.03	Joback Method
cpg	363.66	J/mol×K	587.30	Joback Method
cpg	377.04	J/mol×K	622.57	Joback Method
cpg	389.59	J/mol×K	657.85	Joback Method
cpg	401.54	J/mol×K	693.12	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=R325558&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
ripol:	Polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume