2,6,6-Trimethylcyclohexa-1,4-dienecarbaldehyde

Inchi: InChI=1S/C10H14O/c1-8-5-4-6-10(2,3)9(8)7-11/h4,6-7H,5H2,1-3H3
InchiKey: AXVHXJQWKAFHQW-UHFFFAOYSA-N
Formula: C10H14O
SMILES: CC1=C(C=O)C(C)(C)C=CC1
Mol. weight [g/mol]: 150.22
CAS: 162376-82-1

Physical Properties

Property code	Value	Unit	Source
gf	-6.58	kJ/mol	Joback Method
hf	-173.13	kJ/mol	Joback Method
hfus	11.15	kJ/mol	Joback Method
hvap	45.76	kJ/mol	Joback Method
log10ws	-2.65		Crippen Method
logp	2.488		Crippen Method
mcvol	133.870	ml/mol	McGowan Method
pc	3045.68	kPa	Joback Method
rinpol	1108.70		NIST Webbook
tb	504.93	K	Joback Method
tc	722.27	K	Joback Method
tf	302.30	K	Joback Method
vc	0.515	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	296.18	J/mol×K	504.93	Joback Method
cpg	310.85	J/mol×K	541.15	Joback Method
cpg	324.56	J/mol×K	577.38	Joback Method
cpg	337.42	J/mol×K	613.60	Joback Method
cpg	349.54	J/mol×K	649.82	Joback Method
cpg	361.03	J/mol×K	686.05	Joback Method
cpg	371.98	J/mol×K	722.27	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C162376821&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

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