1,4,4-Trimethylcyclohex-2-enecarboxylic acid

Inchi: InChI=1S/C10H16O2/c1-9(2)4-6-10(3,7-5-9)8(11)12/h4,6H,5,7H2,1-3H3,(H,11,12)
InchiKey: XHDYNNIVGDPHJJ-UHFFFAOYSA-N
Formula: C10H16O2
SMILES: CC1(C)C=CC(C)(C(=O)O)CC1
Mol. weight [g/mol]: 168.23
CAS: 103262-04-0

Physical Properties

Property code	Value	Unit	Source
gf	-196.70	kJ/mol	Joback Method
hf	-392.30	kJ/mol	Joback Method
hfus	8.88	kJ/mol	Joback Method
hvap	59.39	kJ/mol	Joback Method
log10ws	-2.37		Crippen Method
logp	2.454		Crippen Method
mcvol	144.040	ml/mol	McGowan Method
pc	3360.64	kPa	Joback Method
tb	588.77	K	Joback Method
tc	799.36	K	Joback Method
tf	364.91	K	Joback Method
vc	0.534	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	369.52	J/mol×K	588.77	Joback Method
cpg	383.29	J/mol×K	623.87	Joback Method
cpg	396.27	J/mol×K	658.97	Joback Method
cpg	408.65	J/mol×K	694.07	Joback Method
cpg	420.61	J/mol×K	729.17	Joback Method
cpg	432.31	J/mol×K	764.27	Joback Method
cpg	443.95	J/mol×K	799.36	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C103262040&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
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume