1,3,3-Trimethylcyclohex-1-ene-4-carboxylic acid

Other names: 2,2,4-Trimethylcyclohex-3-ene-1-carboxylic acid
Inchi: InChI=1S/C10H16O2/c1-7-4-5-8(9(11)12)10(2,3)6-7/h6,8H,4-5H2,1-3H3,(H,11,12)
InchiKey: LMQGITVNFNTYPJ-UHFFFAOYSA-N
Formula: C10H16O2
SMILES: CC1=CC(C)(C)C(C(=O)O)CC1
Mol. weight [g/mol]: 168.23
CAS: 13746-43-5

Physical Properties

Property code	Value	Unit	Source
gf	-200.84	kJ/mol	Joback Method
hf	-419.01	kJ/mol	Joback Method
hfus	14.78	kJ/mol	Joback Method
hvap	61.20	kJ/mol	Joback Method
log10ws	-2.37		Crippen Method
logp	2.454		Crippen Method
mcvol	144.040	ml/mol	McGowan Method
pc	3138.51	kPa	Joback Method
rinpol	1301.70		NIST Webbook
rinpol	1301.70		NIST Webbook
tb	593.51	K	Joback Method
tc	797.37	K	Joback Method
tf	353.53	K	Joback Method
vc	0.536	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	370.88	J/mol×K	593.51	Joback Method
cpg	384.77	J/mol×K	627.49	Joback Method
cpg	397.93	J/mol×K	661.46	Joback Method
cpg	410.44	J/mol×K	695.44	Joback Method
cpg	422.39	J/mol×K	729.41	Joback Method
cpg	433.86	J/mol×K	763.39	Joback Method

cpg	444.93	J/mol×K	797.37	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=C13746435&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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume