1,3,3-Trimethylcyclohex-1-ene-4-carboxaldehyde, (+,-)-

Other names: 2,2,4-Trimethyl-3-cyclohexene-1-carboxaldehyde
Inchi: InChI=1S/C10H16O/c1-8-4-5-9(7-11)10(2,3)6-8/h6-7,9H,4-5H2,1-3H3
InchiKey: FDSNFOIVNIUNDP-UHFFFAOYSA-N
Formula: C10H16O
SMILES: CC1=CC(C)(C)C(C=O)CC1
Mol. weight [g/mol]: 152.23
CAS: 127128-60-3

Physical Properties

Property code	Value	Unit	Source
gf	-34.62	kJ/mol	Joback Method
hf	-239.78	kJ/mol	Joback Method
hfus	11.39	kJ/mol	Joback Method
hvap	44.50	kJ/mol	Joback Method
log10ws	-2.55		Crippen Method
logp	2.568		Crippen Method
mcvol	138.170	ml/mol	McGowan Method
pc	2871.95	kPa	Joback Method
rinpol	1138.00		NIST Webbook
rinpol	1138.00		NIST Webbook
tb	496.12	K	Joback Method
tc	709.88	K	Joback Method
tf	284.78	K	Joback Method
vc	0.528	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	313.56	J/mol×K	496.12	Joback Method
cpg	330.31	J/mol×K	531.75	Joback Method
cpg	346.01	J/mol×K	567.37	Joback Method
cpg	360.76	J/mol×K	603.00	Joback Method
cpg	374.68	J/mol×K	638.62	Joback Method
cpg	387.85	J/mol×K	674.25	Joback Method

cpg	400.37	J/mol×K	709.88	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C127128603&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

Latest version available from:
https://www.chemeo.com/cid/79-662-0/1-3-3-Trimethylcyclohex-1-ene-4-carboxaldehyde.pdf
Generated by Cheméo on 2024-04-29 11:32:56.970592406 +0000 UTC m=+16679625.891169722.
Cheméo (https://www.chemeo.com) is the biggest free database of chemical and physical data for the process industry.