2,2-dimethylcyclohexane-1-carboxaldehyde

Inchi: InChI=1S/C9H16O/c1-9(2)6-4-3-5-8(9)7-10/h7-8H,3-6H2,1-2H3
InchiKey: PRMCTXHFPWJOSP-UHFFFAOYSA-N
Formula: C9H16O
SMILES: CC1(C)CCCCC1C=O
Mol. weight [g/mol]: 140.22

Physical Properties

Property code	Value	Unit	Source
gf	-63.37	kJ/mol	Joback Method
hf	-265.45	kJ/mol	Joback Method
hfus	7.96	kJ/mol	Joback Method
hvap	41.32	kJ/mol	Joback Method
log10ws	-2.28		Crippen Method
logp	2.402		Crippen Method
mcvol	128.380	ml/mol	McGowan Method
pc	3117.52	kPa	Joback Method
rinpol	1005.00		NIST Webbook
rinpol	1005.00		NIST Webbook
tb	469.10	K	Joback Method
tc	682.62	K	Joback Method
tf	260.23	K	Joback Method
vc	0.486	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	283.87	J/mol×K	469.10	Joback Method
cpg	301.53	J/mol×K	504.69	Joback Method
cpg	318.03	J/mol×K	540.27	Joback Method
cpg	333.50	J/mol×K	575.86	Joback Method
cpg	348.02	J/mol×K	611.45	Joback Method
cpg	361.70	J/mol×K	647.03	Joback Method
cpg	374.64	J/mol×K	682.62	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=R406969&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

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