«gamma»-Campholenic aldehyde

Inchi: InChI=1S/C10H16O/c1-8-4-5-9(6-7-11)10(8,2)3/h7,9H,1,4-6H2,2-3H3
InchiKey: QIMUYKYZQUADBG-UHFFFAOYSA-N
Formula: C10H16O
SMILES: C=C1CCC(CC=O)C1(C)C
Mol. weight [g/mol]: 152.23

Physical Properties

Property code	Value	Unit	Source
gf	10.23	kJ/mol	Joback Method
hf	-195.69	kJ/mol	Joback Method
hfus	11.49	kJ/mol	Joback Method
hvap	43.53	kJ/mol	Joback Method
log10ws	-2.55		Crippen Method
logp	2.568		Crippen Method
mcvol	138.170	ml/mol	McGowan Method
pc	2790.61	kPa	Joback Method
ripol	1435.00		NIST Webbook
ripol	1435.00		NIST Webbook
tb	486.87	K	Joback Method
tc	691.34	K	Joback Method
tf	288.70	K	Joback Method
vc	0.534	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	312.53	J/mol×K	486.87	Joback Method
cpg	328.50	J/mol×K	520.95	Joback Method
cpg	343.49	J/mol×K	555.03	Joback Method
cpg	357.59	J/mol×K	589.10	Joback Method
cpg	370.89	J/mol×K	623.18	Joback Method
cpg	383.49	J/mol×K	657.26	Joback Method
cpg	395.47	J/mol×K	691.34	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R610103&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
ripol:	Polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume