«alpha»-Campholene aldehyde

Inchi: InChI=1S/C10H16O/c1-8-4-5-9(6-7-11)10(8,2)3/h4,7,9H,5-6H2,1-3H3
InchiKey: OGCGGWYLHSJRFY-UHFFFAOYSA-N
Formula: C10H16O
SMILES: CC1=CCC(CC=O)C1(C)C
Mol. weight [g/mol]: 152.23
CAS: 26882-03-1

Physical Properties

Property code	Value	Unit	Source
gf	-22.52	kJ/mol	Joback Method
hf	-233.62	kJ/mol	Joback Method
hfus	13.49	kJ/mol	Joback Method
hvap	44.33	kJ/mol	Joback Method
log10ws	-2.55		Crippen Method
logp	2.568		Crippen Method
mcvol	138.170	ml/mol	McGowan Method
pc	2796.51	kPa	Joback Method
rinpol	1119.00		NIST Webbook
tb	491.85	K	Joback Method
tc	697.74	K	Joback Method
tf	288.30	K	Joback Method
vc	0.536	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	313.66	J/mol×K	491.85	Joback Method
cpg	329.44	J/mol×K	526.17	Joback Method
cpg	344.24	J/mol×K	560.48	Joback Method
cpg	358.15	J/mol×K	594.80	Joback Method
cpg	371.28	J/mol×K	629.11	Joback Method
cpg	383.72	J/mol×K	663.43	Joback Method
cpg	395.56	J/mol×K	697.74	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C26882031&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