«alpha»-Campholenal

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: 91819-58-8

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	1136.00		NIST Webbook
rinpol	1123.00		NIST Webbook
rinpol	1134.00		NIST Webbook
rinpol	1103.00		NIST Webbook
rinpol	1130.00		NIST Webbook
rinpol	1130.00		NIST Webbook
rinpol	1124.00		NIST Webbook
rinpol	1123.00		NIST Webbook
rinpol	1125.00		NIST Webbook
rinpol	1111.00		NIST Webbook
rinpol	1132.00		NIST Webbook
rinpol	1130.00		NIST Webbook
rinpol	1130.00		NIST Webbook
rinpol	1098.00		NIST Webbook
rinpol	1126.00		NIST Webbook
rinpol	1125.00		NIST Webbook
rinpol	1127.00		NIST Webbook
rinpol	1128.00		NIST Webbook
rinpol	1136.00		NIST Webbook
rinpol	1098.00		NIST Webbook

rinpol	1127.00		NIST Webbook
rinpol	1134.00		NIST Webbook
ripol	1489.00		NIST Webbook
ripol	1500.00		NIST Webbook
ripol	1489.00		NIST Webbook
ripol	1486.00		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

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C91819588&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
rinpol:	Non-polar retention indices
ripol:	Polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume