«alpha»-Campholenol

Other names: «alpha»-Campholene alcohol
2,2,3-Trimethyl-cyclopent-3-ene,1-ethanol
campholene alcohol
Inchi: InChI=1S/C10H18O/c1-8-4-5-9(6-7-11)10(8,2)3/h4,9,11H,5-7H2,1-3H3
InchiKey: NPGPPCSBEMHHCR-UHFFFAOYSA-N
Formula: C10H18O
SMILES: CC1=CCC(CCO)C1(C)C
Mol. weight [g/mol]: 154.25
CAS: 1901-38-8

Physical Properties

Property code	Value	Unit	Source
gf	-59.82	kJ/mol	Joback Method
hf	-300.27	kJ/mol	Joback Method
hfus	15.28	kJ/mol	Joback Method
hvap	54.28	kJ/mol	Joback Method
log10ws	-2.54		Crippen Method
logp	2.361		Crippen Method
mcvol	142.470	ml/mol	McGowan Method
pc	2850.52	kPa	Joback Method
rinpol	1185.00		NIST Webbook
rinpol	1185.00		NIST Webbook
rinpol	1186.00		NIST Webbook
rinpol	1202.00		NIST Webbook
ripol	1790.00		NIST Webbook
ripol	1805.00		NIST Webbook
ripol	1805.00		NIST Webbook
ripol	1782.00		NIST Webbook
ripol	1800.00		NIST Webbook
ripol	1800.00		NIST Webbook
ripol	1782.00		NIST Webbook
ripol	1790.00		NIST Webbook
tb	535.37	K	Joback Method
tc	724.71	K	Joback Method
tf	307.12	K	Joback Method
vc	0.538	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	350.35	J/mol×K	535.37	Joback Method
cpg	364.68	J/mol×K	566.93	Joback Method
cpg	378.25	J/mol×K	598.48	Joback Method
cpg	391.13	J/mol×K	630.04	Joback Method
cpg	403.40	J/mol×K	661.59	Joback Method
cpg	415.13	J/mol×K	693.15	Joback Method
cpg	426.40	J/mol×K	724.71	Joback Method

Sources

McGowan Method: http://link.springer.com/article/10.1007/BF02311772
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C1901388&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
ripol: Polar retention indices
tb: Normal Boiling Point Temperature
tc: Critical Temperature

tf: Normal melting (fusion) point

vc: Critical Volume