Photonerol

Inchi: InChI=1S/C10H18O/c1-9(2)7-4-5-10(7,3)8(9)6-11/h7-8,11H,4-6H2,1-3H3
InchiKey: ZCZAIJOOJJJLON-UHFFFAOYSA-N
Formula: C10H18O
SMILES: CC1(C)C(CO)C2(C)CCC12
Mol. weight [g/mol]: 154.25

Physical Properties

Property code	Value	Unit	Source
gf	-8.40	kJ/mol	Joback Method
hf	-266.56	kJ/mol	Joback Method
hfus	11.56	kJ/mol	Joback Method
hvap	51.44	kJ/mol	Joback Method
log10ws	-2.09		Crippen Method
logp	2.051		Crippen Method
mcvol	135.910	ml/mol	McGowan Method
pc	3079.57	kPa	Joback Method
rinpol	1215.00		NIST Webbook
tb	525.00	K	Joback Method
tc	719.05	K	Joback Method
tf	338.48	K	Joback Method
vc	0.522	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	353.88	J/mol×K	525.00	Joback Method
cpg	368.98	J/mol×K	557.34	Joback Method
cpg	383.01	J/mol×K	589.68	Joback Method
cpg	396.13	J/mol×K	622.02	Joback Method
cpg	408.53	J/mol×K	654.36	Joback Method
cpg	420.37	J/mol×K	686.70	Joback Method
cpg	431.83	J/mol×K	719.05	Joback Method

Sources

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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R513092&Units=SI

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