Oxycitronellol

Inchi: InChI=1S/C10H20O2/c1-8(2)6-10(12)7-9(3)4-5-11/h6,9-12H,4-5,7H2,1-3H3
InchiKey: JMXVHRVVQNPWNN-UHFFFAOYSA-N
Formula: C10H20O2
SMILES: CC(C)=CC(O)CC(C)CCO
Mol. weight [g/mol]: 172.26

Physical Properties

Property code	Value	Unit	Source
gf	-173.53	kJ/mol	Joback Method
hf	-457.32	kJ/mol	Joback Method
hfus	21.68	kJ/mol	Joback Method
hvap	70.47	kJ/mol	Joback Method
log10ws	-2.26		Crippen Method
logp	1.722		Crippen Method
mcvol	159.200	ml/mol	McGowan Method
pc	2709.85	kPa	Joback Method
rinpol	1347.00		NIST Webbook
rinpol	1347.00		NIST Webbook
ripol	2143.00		NIST Webbook
tb	615.72	K	Joback Method
tc	784.20	K	Joback Method
tf	275.06	K	Joback Method
vc	0.603	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	421.50	J/mol×K	615.72	Joback Method
cpg	433.13	J/mol×K	643.80	Joback Method
cpg	444.24	J/mol×K	671.88	Joback Method
cpg	454.84	J/mol×K	699.96	Joback Method
cpg	464.96	J/mol×K	728.04	Joback Method
cpg	474.62	J/mol×K	756.12	Joback Method
cpg	483.85	J/mol×K	784.20	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R410121&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