neral propylene glycol acetal (isomer)

Inchi: InChI=1S/C14H24O2/c1-11(2)6-5-7-12(3)8-9-14-15-10-13(4)16-14/h6,8,13-14H,5,7,9-10
InchiKey: SOLUPKFWUPOIEI-WQLSENKSSA-N
Formula: C14H24O2
SMILES: CC(C)=CCCC(C)=CCC1OCC(C)O1
Mol. weight [g/mol]: 224.34

Physical Properties

Property code	Value	Unit	Source
gf	66.94	kJ/mol	Joback Method
hf	-341.29	kJ/mol	Joback Method
hfus	40.76	kJ/mol	Joback Method
hvap	55.80	kJ/mol	Joback Method
log10ws	-4.18		Crippen Method
logp	3.831		Crippen Method
mcvol	200.400	ml/mol	McGowan Method
pc	1859.51	kPa	Joback Method
ripol	1836.00		NIST Webbook
ripol	1847.00		NIST Webbook
ripol	1836.00		NIST Webbook
tb	592.31	K	Joback Method
tc	794.04	K	Joback Method
tf	269.26	K	Joback Method
vc	0.763	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	531.62	J/mol×K	592.31	Joback Method
cpg	551.33	J/mol×K	625.93	Joback Method
cpg	569.94	J/mol×K	659.55	Joback Method
cpg	587.49	J/mol×K	693.18	Joback Method
cpg	604.05	J/mol×K	726.80	Joback Method
cpg	619.68	J/mol×K	760.42	Joback Method
cpg	634.43	J/mol×K	794.04	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=R441640&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
ripol:	Polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume