Cedrane, 8-propoxy-

Other names: Cedryl propyl ether
8-propoxycedrane
Inchi: InChI=1S/C18H32O/c1-6-11-19-17(5)9-10-18-12-15(17)16(3,4)14(18)8-7-13(18)2/h13-15
InchiKey: TUDJGTBGFVLELQ-UHFFFAOYSA-N
Formula: C18H32O
SMILES: CCCOC1(C)CCC23CC1C(C)(C)C2CCC3C
Mol. weight [g/mol]: 264.45
CAS: 19870-75-8

Physical Properties

Property code	Value	Unit	Source
gf	114.13	kJ/mol	Joback Method
hf	-356.29	kJ/mol	Joback Method
hfus	18.09	kJ/mol	Joback Method
hvap	53.78	kJ/mol	Joback Method
log10ws	-5.03		Crippen Method
logp	5.044		Crippen Method
mcvol	237.770	ml/mol	McGowan Method
pc	1616.77	kPa	Joback Method
rinpol	1652.00		NIST Webbook
rinpol	1652.00		NIST Webbook
tb	649.13	K	Joback Method
tc	865.35	K	Joback Method
tf	420.61	K	Joback Method
vc	0.907	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	717.42	J/mol×K	649.13	Joback Method
cpg	742.03	J/mol×K	685.17	Joback Method
cpg	765.63	J/mol×K	721.20	Joback Method
cpg	788.57	J/mol×K	757.24	Joback Method
cpg	811.18	J/mol×K	793.27	Joback Method

cpg	833.79	J/mol×K	829.31	Joback Method
cpg	856.74	J/mol×K	865.35	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C19870758&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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume