Panaxydol

Inchi: InChI=1S/C17H24O2/c1-3-5-6-7-10-13-16-17(19-16)14-11-8-9-12-15(18)4-2/h4,15-18H,2
InchiKey: GVLDSGIQZAFIAN-UHFFFAOYSA-N
Formula: C17H24O2
SMILES: C=CC(O)C#CC#CCC1OC1CCCCCCC
Mol. weight [g/mol]: 260.37
CAS: 72800-72-7

Physical Properties

Property code	Value	Unit	Source
gf	413.36	kJ/mol	Joback Method
hf	38.77	kJ/mol	Joback Method
hfus	52.50	kJ/mol	Joback Method
hvap	77.47	kJ/mol	Joback Method
log10ws	-4.96		Crippen Method
logp	3.058		Crippen Method
mcvol	229.770	ml/mol	McGowan Method
pc	1890.36	kPa	Joback Method
rinpol	2192.80		NIST Webbook
rinpol	2192.80		NIST Webbook
tb	723.80	K	Joback Method
tc	922.40	K	Joback Method
tf	577.88	K	Joback Method
vc	0.882	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	659.49	J/mol×K	723.80	Joback Method
cpg	675.50	J/mol×K	756.90	Joback Method
cpg	690.68	J/mol×K	790.00	Joback Method
cpg	705.06	J/mol×K	823.10	Joback Method
cpg	718.72	J/mol×K	856.20	Joback Method
cpg	731.68	J/mol×K	889.30	Joback Method
cpg	744.02	J/mol×K	922.40	Joback Method

Sources

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=C72800727&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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