Ginsenoyne E

Inchi: InChI=1S/C17H22O2/c1-3-5-6-7-10-13-16-17(19-16)14-11-8-9-12-15(18)4-2/h4,16-17H,2
InchiKey: WIONCQLWGYLTME-UHFFFAOYSA-N
Formula: C17H22O2
SMILES: C=CC(=O)C#CC#CCC1OC1CCCCCCC
Mol. weight [g/mol]: 258.36
CAS: 126146-63-2

Physical Properties

Property code	Value	Unit	Source
gf	423.70	kJ/mol	Joback Method
hf	83.70	kJ/mol	Joback Method
hfus	53.53	kJ/mol	Joback Method
hvap	67.93	kJ/mol	Joback Method
log10ws	-4.87		Crippen Method
logp	3.266		Crippen Method
mcvol	225.470	ml/mol	McGowan Method
pc	1830.98	kPa	Joback Method
rinpol	2160.00		NIST Webbook
rinpol	2160.00		NIST Webbook
tb	685.93	K	Joback Method
tc	898.85	K	Joback Method
tf	581.99	K	Joback Method
vc	0.875	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	615.93	J/mol×K	685.93	Joback Method
cpg	633.40	J/mol×K	721.42	Joback Method
cpg	649.87	J/mol×K	756.90	Joback Method
cpg	665.40	J/mol×K	792.39	Joback Method
cpg	680.05	J/mol×K	827.88	Joback Method
cpg	693.89	J/mol×K	863.36	Joback Method
cpg	706.96	J/mol×K	898.85	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=C126146632&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