«tau»-Stearolactone

Inchi: InChI=1S/C18H34O2/c1-2-3-4-5-6-7-8-9-10-11-12-14-17-15-13-16-18(19)20-17/h17H,2-1
InchiKey: VVLRVPJYFLFSQG-UHFFFAOYSA-N
Formula: C18H34O2
SMILES: CCCCCCCCCCCCCCC1CCCC(=O)O1
Mol. weight [g/mol]: 282.46

Physical Properties

Property code	Value	Unit	Source
af	0.8244		Cheméo Relay (1.0)
gf	-83.58	kJ/mol	Joback Method
hf	-680.09	kJ/mol	Cheméo Relay (1.0)
hfus	41.70	kJ/mol	Joback Method
hvap	104.14	kJ/mol	Cheméo Relay (1.0)
ie	9.87	eV	Cheméo Relay (1.0)
logp	5.783		Crippen Method
mcvol	261.060	ml/mol	McGowan Method
pc	1356.63	kPa	Joback Method
rinpol	2196.00		NIST Webbook
rinpol	2196.00		NIST Webbook
rinpol	2196.00		NIST Webbook
tb	642.84	K	Cheméo Relay (1.0)
tc	822.28	K	Cheméo Relay (1.0)
tf	303.47	K	Cheméo Relay (1.0)
vc	0.996	m3/kmol	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	807.34	J/mol×K	725.56	Joback Method
cpg	828.45	J/mol×K	757.55	Joback Method
cpg	848.39	J/mol×K	789.53	Joback Method
cpg	867.18	J/mol×K	821.52	Joback Method
cpg	884.84	J/mol×K	853.50	Joback Method
cpg	901.37	J/mol×K	885.49	Joback Method

cpg	916.81	J/mol×K	917.48	Joback Method

Sources

Cheméo Relay (1.0):

Cheméo Relay (1.0, beta):

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=R613211&Units=SI

Joback Method: https://en.wikipedia.org/wiki/Joback_method

McGowan Method: http://link.springer.com/article/10.1007/BF02311772

Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws

Legend

af: Acentric Factor
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
ie: Ionization energy
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