Nezukol

Inchi: InChI=1S/C20H34O/c1-6-18(4)12-8-16-19(5)11-7-10-17(2,3)15(19)9-13-20(16,21)14-18/
InchiKey: IYDAPILQPCDHTO-XZJNCXDESA-N
Formula: C20H34O
SMILES: C=CC1(C)CCC2C(O)(CCC3C(C)(C)CCCC32C)C1
Mol. weight [g/mol]: 290.48
CAS: 14699-32-2

Physical Properties

Property code	Value	Unit	Source
gf	145.20	kJ/mol	Joback Method
hf	-295.39	kJ/mol	Joback Method
hfus	12.29	kJ/mol	Joback Method
hvap	71.19	kJ/mol	Joback Method
log10ws	-5.90		Crippen Method
logp	5.336		Crippen Method
mcvol	261.650	ml/mol	McGowan Method
pc	1724.59	kPa	Joback Method
rinpol	2080.00		NIST Webbook
rinpol	2133.00		NIST Webbook
rinpol	2130.00		NIST Webbook
rinpol	2126.00		NIST Webbook
rinpol	2126.00		NIST Webbook
rinpol	2133.00		NIST Webbook
rinpol	2134.00		NIST Webbook
tb	774.38	K	Joback Method
tc	1000.33	K	Joback Method
tf	493.32	K	Joback Method
vc	0.976	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	865.79	J/mol×K	774.38	Joback Method
cpg	891.86	J/mol×K	812.04	Joback Method

cpg	918.41	J/mol×K	849.70	Joback Method
cpg	945.91	J/mol×K	887.36	Joback Method
cpg	974.86	J/mol×K	925.01	Joback Method
cpg	1005.73	J/mol×K	962.67	Joback Method
cpg	1039.02	J/mol×K	1000.33	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=C14699322&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
rinpol: Non-polar retention indices
tb: Normal Boiling Point Temperature
tc: Critical Temperature
tf: Normal melting (fusion) point
vc: Critical Volume