Urs-12-ene

Inchi: InChI=1S/C30H50/c1-20-12-16-27(5)18-19-29(7)22(25(27)21(20)2)10-11-24-28(6)15-9-1
InchiKey: DGXIUFDVYPIXCI-UHFFFAOYSA-N
Formula: C30H50
SMILES: CC1CCC2(C)CCC3(C)C(=CCC4C5(C)CCCC(C)(C)C5CCC43C)C2C1C
Mol. weight [g/mol]: 410.72
CAS: 464-97-1

Physical Properties

Property code	Value	Unit	Source
gf	375.10	kJ/mol	Joback Method
hf	-320.84	kJ/mol	Joback Method
hfus	24.13	kJ/mol	Joback Method
hvap	76.80	kJ/mol	Joback Method
log10ws	-9.29		Crippen Method
logp	9.054		Crippen Method
mcvol	374.960	ml/mol	McGowan Method
pc	981.46	kPa	Joback Method
rinpol	5002.00		NIST Webbook
rinpol	5002.00		NIST Webbook
tb	931.38	K	Joback Method
tc	1179.69	K	Joback Method
tf	604.50	K	Joback Method
vc	1.415	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1432.64	J/mol×K	931.38	Joback Method
cpg	1480.45	J/mol×K	972.76	Joback Method
cpg	1531.81	J/mol×K	1014.15	Joback Method
cpg	1587.53	J/mol×K	1055.53	Joback Method
cpg	1648.46	J/mol×K	1096.92	Joback Method
cpg	1715.43	J/mol×K	1138.30	Joback Method
cpg	1789.28	J/mol×K	1179.69	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C464971&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