Urs-12-en-28-al, 3-(acetyloxy)-, (3«beta»)-

Other names: 3«beta»-Acetoxyurs-12-en-28-al
Inchi: InChI=1S/C32H50O3/c1-20-11-16-32(19-33)18-17-30(7)23(27(32)21(20)2)9-10-25-29(6)
InchiKey: RVSZZPCRCJYAEU-UHFFFAOYSA-N
Formula: C32H50O3
SMILES: CC(=O)OC1CCC2(C)C(CCC3(C)C2CC=C2C4C(C)C(C)CCC4(C=O)CCC23C)C1(C)C
Mol. weight [g/mol]: 482.74
CAS: 86996-88-5

Physical Properties

Property code	Value	Unit	Source
gf	50.79	kJ/mol	Joback Method
hf	-712.84	kJ/mol	Joback Method
hfus	35.46	kJ/mol	Joback Method
hvap	96.82	kJ/mol	Joback Method
log10ws	-8.38		Crippen Method
logp	7.775		Crippen Method
mcvol	412.150	ml/mol	McGowan Method
pc	919.95	kPa	Joback Method
rinpol	3727.00		NIST Webbook
rinpol	3727.00		NIST Webbook
tb	1097.42	K	Joback Method
tc	1351.73	K	Joback Method
tf	736.96	K	Joback Method
vc	1.567	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1756.33	J/mol×K	1097.42	Joback Method
cpg	1823.77	J/mol×K	1139.80	Joback Method
cpg	1897.89	J/mol×K	1182.19	Joback Method
cpg	1979.56	J/mol×K	1224.57	Joback Method
cpg	2069.62	J/mol×K	1266.96	Joback Method
cpg	2168.96	J/mol×K	1309.34	Joback Method

cpg	2278.43	J/mol×K	1351.73	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C86996885&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