4-Campestene-3-one

Inchi: InChI=1S/C28H46O/c1-18(2)19(3)7-8-20(4)24-11-12-25-23-10-9-21-17-22(29)13-15-27(2
InchiKey: QQIOPZFVTIHASB-XGKIWTSOSA-N
Formula: C28H46O
SMILES: CC(C)C(C)CCC(C)C1CCC2C3CCC4=CC(=O)CCC4(C)C3CCC12C
Mol. weight [g/mol]: 398.66
CAS: 51014-22-3

Physical Properties

Property code	Value	Unit	Source
gf	231.40	kJ/mol	Joback Method
hf	-478.28	kJ/mol	Joback Method
hfus	29.64	kJ/mol	Joback Method
hvap	79.55	kJ/mol	Joback Method
log10ws	-8.08		Crippen Method
logp	7.843		Crippen Method
mcvol	359.210	ml/mol	McGowan Method
pc	1003.35	kPa	Joback Method
rinpol	3370.70		NIST Webbook
rinpol	3370.70		NIST Webbook
tb	950.13	K	Joback Method
tc	1185.11	K	Joback Method
tf	535.30	K	Joback Method
vc	1.361	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1344.94	J/mol×K	950.13	Joback Method
cpg	1377.23	J/mol×K	989.29	Joback Method
cpg	1409.84	J/mol×K	1028.46	Joback Method
cpg	1443.11	J/mol×K	1067.62	Joback Method
cpg	1477.40	J/mol×K	1106.78	Joback Method
cpg	1513.06	J/mol×K	1145.94	Joback Method
cpg	1550.44	J/mol×K	1185.11	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C51014223&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

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