

Castasterone

Inchi: InChI=1S/C28H48O5/c1-14(2)15(3)25(32)26(33)16(4)18-7-8-19-17-11-22(29)21-12-23(3)
InchiKey: VYUIKSFYFRVQLF-LXNWWJPRTSA-N
Formula: C28H48O5
SMILES: CC(C)C(C)C(O)C(O)C(C)C1CCC2C3CC(=O)C4CC(O)C(O)CC4(C)C3CCC12C
Mol. weight [g/mol]: 464.68

Physical Properties

Property code	Value	Unit	Source
gf	-364.22	kJ/mol	Joback Method
hf	-1205.09	kJ/mol	Joback Method
hfus	41.32	kJ/mol	Joback Method
hvap	143.61	kJ/mol	Joback Method
log10ws	-5.49		Crippen Method
logp	3.806		Crippen Method
mcvol	386.990	ml/mol	McGowan Method
pc	1194.82	kPa	Joback Method
rinpol	3630.00		NIST Webbook
rinpol	3630.00		NIST Webbook
tb	1299.82	K	Joback Method
tc	1651.65	K	Joback Method
tf	722.58	K	Joback Method
vc	1.435	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1798.92	J/mol×K	1299.82	Joback Method
cpg	1867.66	J/mol×K	1358.46	Joback Method
cpg	1943.52	J/mol×K	1417.10	Joback Method
cpg	2027.64	J/mol×K	1475.74	Joback Method
cpg	2121.18	J/mol×K	1534.38	Joback Method
cpg	2225.28	J/mol×K	1593.01	Joback Method
cpg	2341.09	J/mol×K	1651.65	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R553436&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
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
hvp:	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
rinp:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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