

Beclomethasone

Other names:	Pregna-1,4-diene-3,20-dione, 9-chloro-11,17,21-trihydroxy-16-methyl-, (11«beta»,16«beta»)- 9-Chloro-11«beta»,17,21-trihydroxy-16«beta»-methyl-pregna-1,4-diene-3,20-dione 9«alpha»-Chloro-16«beta»-methylprednisolone Beclometasone
Inchi:	InChI=1S/C22H29ClO5/c1-12-8-16-15-5-4-13-9-14(25)6-7-19(13,2)21(15,23)17(26)10-20
InchiKey:	NBMKJKDGKREAPL-UHFFFAOYSA-N
Formula:	C22H29ClO5
SMILES:	CC1CC2C3CCC4=CC(=O)C=CC4(C)C3(Cl)C(O)CC2(C)C1(O)C(=O)CO
Mol. weight [g/mol]:	408.92
CAS:	4419-39-0

Physical Properties

Property code	Value	Unit	Source
gf	-359.55	kJ/mol	Joback Method
hf	-876.03	kJ/mol	Joback Method
hfus	33.49	kJ/mol	Joback Method
hvap	125.90	kJ/mol	Joback Method
log10ws	-3.95		Crippen Method
logp	2.165		Crippen Method
mcvol	301.790	ml/mol	McGowan Method
pc	1987.66	kPa	Joback Method
tb	1172.31	K	Joback Method
tc	1436.12	K	Joback Method
tf	815.07	K	Joback Method
vc	1.135	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1317.36	J/mol×K	1172.31	Joback Method
cpg	1380.91	J/mol×K	1216.28	Joback Method
cpg	1451.82	J/mol×K	1260.25	Joback Method
cpg	1530.84	J/mol×K	1304.21	Joback Method
cpg	1618.73	J/mol×K	1348.18	Joback Method

cpg	1716.24	J/mol×K	1392.15	Joback Method
cpg	1824.13	J/mol×K	1436.12	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C4419390&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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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