

Etoposide (148-167,25mg/ml)

Inchi:	InChI=1S/C29H32O13/c1-11-36-9-20-27(40-11)24(31)25(32)29(41-20)42-26-14-7-17-16
InchiKey:	VJJPUSNTGOMMGY-UHFFFAOYSA-N
Formula:	C29H32O13
SMILES:	<chem>COc1cc(C2c3cc4c(cc3C(OC3OC5COC(C)OC5C(O)C3O)C3COC(=O)C23)OCO4)cc(OC</chem>
Mol. weight [g/mol]:	588.56

Physical Properties

Property code	Value	Unit	Source
gf	-807.90	kJ/mol	Joback Method
hf	-1802.81	kJ/mol	Joback Method
hfus	107.44	kJ/mol	Joback Method
hvap	171.80	kJ/mol	Joback Method
log10ws	-3.57		Estimated Solubility Method
log10ws	-3.57		Aqueous Solubility Prediction Method
logp	1.339		Crippen Method
mcvol	389.660	ml/mol	McGowan Method
pc	1547.57	kPa	Joback Method
tb	1534.64	K	Joback Method
tc	1946.74	K	Joback Method
tf	516.65	K	Aqueous Solubility Prediction Method
vc	1.375	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1575.93	J/molxK	1534.64	Joback Method
cpg	1580.20	J/molxK	1603.32	Joback Method
cpg	1583.19	J/molxK	1672.01	Joback Method
cpg	1585.43	J/molxK	1740.69	Joback Method
cpg	1587.51	J/molxK	1809.37	Joback Method
cpg	1589.99	J/molxK	1878.06	Joback Method
cpg	1593.41	J/molxK	1946.74	Joback Method

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
Aqueous Solubility Prediction Method:	http://onschallenge.wikispaces.com/file/view/AqueousDataset002.xlsx/351826032/AqueousDa
Estimated Solubility Method:	http://pubs.acs.org/doi/suppl/10.1021/ci034243x/suppl_file/ci034243xsi20040112_053635.txt
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
h vap:	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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