Erythromycin, ethyl carbonate

Inchi: InChI=1S/C40H71NO15/c1-15-27-40(11,48)32(43)22(5)29(42)20(3)18-38(9,47)34(56-36
InchiKey: BSUQCLSFQSUNED-UHFFFAOYSA-N
Formula: C40H71NO15
SMILES: CCOC(=O)OC1C(OC2C(C)C(OC3CC(C)(OC)C(O)C(C)O3)C(C)C(=O)OC(CC)C(C)(O)C(
Mol. weight [g/mol]: 805.99

Physical Properties

Property code	Value	Unit	Source
gf	-1463.61	kJ/mol	Joback Method
hf	-3001.10	kJ/mol	Joback Method
hfus	105.10	kJ/mol	Joback Method
hvap	208.79	kJ/mol	Joback Method
log10ws	-5.97		Crippen Method
logp	2.966		Crippen Method
mcvol	627.010	ml/mol	McGowan Method
pc	562.60	kPa	Joback Method
tb	1901.70	K	Joback Method
tc	3353.93	K	Joback Method
tf	1195.62	K	Joback Method
vc	2.256	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	2700.92	J/mol×K	1901.70	Joback Method
cpg	2615.67	J/mol×K	2143.74	Joback Method
cpg	2506.35	J/mol×K	2385.78	Joback Method
cpg	2395.67	J/mol×K	2627.82	Joback Method
cpg	2306.34	J/mol×K	2869.85	Joback Method
cpg	2261.06	J/mol×K	3111.89	Joback Method
cpg	2282.53	J/mol×K	3353.93	Joback Method

Sources

Joback Method:	https://en.wikipedia.org/wiki/Joback_method
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=B6005035&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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