Glycyrrhizin

Other names:
Inchi: (2S,3S,4S,5R,6R)-6-(((2R,3R,4S,5S,6S)-6-carboxy-2-(((6aR,6bR,8aS,11S,14bS)-11-carb
InChI=1S/C42H62O16/c1-37(2)21-8-11-42(7)31(20(43)16-18-19-17-39(4,36(53)54)13-12
acid
InchiKey: LPLVUJXQOOQHMX-QNEPSFRFSA-N
Formula: C42H62O16
SMILES: CC1(C(=O)O)CCC2(C)CCC3(C)C(=CC(=O)C4C5(C)CCC(OC6OC(C(=O)O)C(O)C(O)C6
Mol. weight [g/mol]: 822.94

Physical Properties

Property code	Value	Unit	Source
hfus	96.49	kJ/mol	Joback Method
logp	2.246		Crippen Method
mcvol	599.040	ml/mol	McGowan Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	9661.64	J/mol×K	2273.53	Joback Method
cpg	28172.42	J/mol×K	3123.70	Joback Method
cpg	66226.52	J/mol×K	3973.87	Joback Method
cpg	131223.55	J/mol×K	4824.03	Joback Method
cpg	230563.10	J/mol×K	5674.20	Joback Method
cpg	371644.77	J/mol×K	6524.37	Joback Method
cpg	561868.15	J/mol×K	7374.54	Joback Method

Sources

Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws
Cheméo Relay (1.0):
Cheméo Relay (1.0, beta):
Solubility of Glycyrrhizin in supercritical carbon dioxide with and without cosolvent: https://www.doi.org/10.1021/je5011328
Joback Method: https://en.wikipedia.org/wiki/Joback_method

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

Legend

cpg:	Ideal gas heat capacity
hfus:	Enthalpy of fusion at standard conditions
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume