

4-(3,7-dihydroxy-10,13-dimethyl-2,3,4,5,6,7,8,9,11,

Inchi:
acid

InChI=1S/C24H40O4/c1-14(4-7-21(27)28)17-5-6-18-22-19(9-11-24(17,18)3)23(2)10-8-16

InchiKey:

RUDATBOHQWOJDD-UHFFFAOYSA-N

Formula:

C24H40O4

SMILES:

CC(CCC(=O)O)C1CCC2C3C(O)CC4CC(O)CCC4(C)C3CCC12C

Mol. weight [g/mol]:

392.58

Physical Properties

Property code	Value	Unit	Source
gf	-257.65	kJ/mol	Joback Method
hf	-924.06	kJ/mol	Joback Method
hfus	43.05	kJ/mol	Joback Method
hvap	122.08	kJ/mol	Joback Method
log10ws	-3.91		Aqueous Solubility Prediction Method
logp	4.478		Crippen Method
mcvol	324.760	ml/mol	McGowan Method
pc	1473.62	kPa	Joback Method
tb	1103.93	K	Joback Method
tc	1355.36	K	Joback Method
tf	658.39	K	Joback Method
vc	1.216	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1362.41	J/molxK	1103.93	Joback Method
cpg	1398.81	J/molxK	1145.83	Joback Method
cpg	1437.44	J/molxK	1187.74	Joback Method
cpg	1478.72	J/molxK	1229.64	Joback Method
cpg	1523.11	J/molxK	1271.55	Joback Method
cpg	1571.04	J/molxK	1313.45	Joback Method
cpg	1622.95	J/molxK	1355.36	Joback Method

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307I
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
Aqueous Solubility Prediction Method:	http://onschallenge.wikispaces.com/file/view/AqueousDataset002.xlsx/351826032/AqueousDa
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
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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