iopromide

Inchi: InChI=1S/C18H24I3N3O8/c1-24(4-9(28)6-26)18(31)12-13(19)11(17(30)22-3-8(27)5-25)1
InchiKey: DGAIEPBNLOQYER-UHFFFAOYSA-N
Formula: C18H24I3N3O8
SMILES: COCC(=O)Nc1c(I)c(C(=O)NCC(O)CO)c(I)c(C(=O)N(C)CC(O)CO)c1I
Mol. weight [g/mol]: 791.12

Physical Properties

Property code	Value	Unit	Source
hfus	76.20	kJ/mol	Joback Method
logp	-0.406		Crippen Method
mcvol	382.180	ml/mol	McGowan Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1129.31	J/mol×K	1606.89	Joback Method
cpg	1144.70	J/mol×K	1702.40	Joback Method
cpg	1162.85	J/mol×K	1797.92	Joback Method
cpg	1185.00	J/mol×K	1893.43	Joback Method
cpg	1212.41	J/mol×K	1988.95	Joback Method
cpg	1246.31	J/mol×K	2084.46	Joback Method
cpg	1287.95	J/mol×K	2179.98	Joback Method

Sources

Cheméo Relay (1.0):

Cheméo Relay (1.0, beta):

Influence of Different Solvent Properties and Composition for the Solubility of Iopromide: https://www.doi.org/10.1021/acs.jced.8b00416

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