iohexol

Inchi: InChI=1S/C19H26I3N3O9/c1-8(29)25(4-11(32)7-28)17-15(21)12(18(33)23-2-9(30)5-26)1
InchiKey: NTHXOOBQLCIOLC-UHFFFAOYSA-N
Formula: C19H26I3N3O9
SMILES: CC(=O)N(CC(O)CO)c1c(I)c(C(=O)NCC(O)CO)c(I)c(C(=O)NCC(O)CO)c1I
Mol. weight [g/mol]: 821.14

Physical Properties

Property code	Value	Unit	Source
hfus	82.26	kJ/mol	Joback Method
logp	-1.627		Crippen Method
mcvol	402.140	ml/mol	McGowan Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1316.76	J/mol×K	1791.27	Joback Method
cpg	1410.85	J/mol×K	1968.37	Joback Method
cpg	1543.74	J/mol×K	2145.46	Joback Method
cpg	1726.24	J/mol×K	2322.56	Joback Method
cpg	1969.15	J/mol×K	2499.66	Joback Method
cpg	2283.27	J/mol×K	2676.75	Joback Method
cpg	2679.41	J/mol×K	2853.85	Joback Method

Sources

Solubility in Different Solvents, Correlation, and Solvent Effect in the Solvent Crystallization Process of Iohexol: https://www.doi.org/10.1021/acs.jced.8b01101
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
Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws
Cheméo Relay (1.0):

Legend

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