L-tyrosine, n-benzoyl-3,5-diiodo-, ethyl ester

Inchi: InChI=1S/C18H17I2NO4/c1-2-25-18(24)15(21-17(23)12-6-4-3-5-7-12)10-11-8-13(19)16(
InchiKey: LMPGZRBXGQHUBL-UHFFFAOYSA-N
Formula: C18H17I2NO4
SMILES: CCOC(=O)C(Cc1cc(I)c(O)c(I)c1)NC(=O)c1ccccc1
Mol. weight [g/mol]: 565.14
CAS: 195067-03-9

Physical Properties

Property code	Value	Unit	Source
gf	-8.03	kJ/mol	Joback Method
hf	-297.49	kJ/mol	Joback Method
hfus	50.24	kJ/mol	Joback Method
hvap	115.25	kJ/mol	Joback Method
log10ws	-5.92		Crippen Method
logp	3.506		Crippen Method
mcvol	293.460	ml/mol	McGowan Method
pc	2313.61	kPa	Joback Method
tb	1121.35	K	Joback Method
tc	1399.80	K	Joback Method
tf	758.09	K	Joback Method
vc	1.028	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	812.38	J/mol×K	1121.35	Joback Method
cpg	824.60	J/mol×K	1167.76	Joback Method
cpg	836.98	J/mol×K	1214.17	Joback Method
cpg	849.72	J/mol×K	1260.57	Joback Method
cpg	863.03	J/mol×K	1306.98	Joback Method
cpg	877.13	J/mol×K	1353.39	Joback Method
cpg	892.23	J/mol×K	1399.80	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C195067039&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Joback Method:	https://en.wikipedia.org/wiki/Joback_method

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