

I-Tyrosine, N,O-bis(4-fluorobenzoyl)-, methyl ester

Inchi:	InChI=1S/C24H19F2NO5/c1-31-24(30)21(27-22(28)16-4-8-18(25)9-5-16)14-15-2-12-20(
InchiKey:	KSGDFDOOYLWHMW-UHFFFAOYSA-N
Formula:	C24H19F2NO5
SMILES:	COC(=O)C(Cc1ccc(OC(=O)c2ccc(F)cc2)cc1)NC(=O)c1ccc(F)cc1
Mol. weight [g/mol]:	439.41

Physical Properties

Property code	Value	Unit	Source
gf	-439.89	kJ/mol	Joback Method
hf	-809.72	kJ/mol	Joback Method
hfus	53.78	kJ/mol	Joback Method
hvap	107.30	kJ/mol	Joback Method
log10ws	-6.41		Crippen Method
logp	3.698		Crippen Method
mcvol	307.710	ml/mol	McGowan Method
pc	1615.47	kPa	Joback Method
tb	1098.22	K	Joback Method
tc	1348.59	K	Joback Method
tf	710.15	K	Joback Method
vc	1.175	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	971.72	J/molxK	1098.22	Joback Method
cpg	978.91	J/molxK	1139.95	Joback Method
cpg	984.61	J/molxK	1181.68	Joback Method
cpg	988.88	J/molxK	1223.41	Joback Method
cpg	991.78	J/molxK	1265.13	Joback Method
cpg	993.39	J/molxK	1306.86	Joback Method
cpg	993.78	J/molxK	1348.59	Joback Method

Sources

Joback Method:	https://en.wikipedia.org/wiki/Joback_method
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U299611&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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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