l-Tyrosine, N,O-bis(butyryl)-, methyl ester

Inchi: InChI=1S/C18H25NO5/c1-4-6-16(20)19-15(18(22)23-3)12-13-8-10-14(11-9-13)24-17(21)
InchiKey: ZZBJAIOUEAXYCC-UHFFFAOYSA-N
Formula: C18H25NO5
SMILES: CCCC(=O)NC(Cc1ccc(OC(=O)CCC)cc1)C(=O)OC
Mol. weight [g/mol]: 335.39

Physical Properties

Property code	Value	Unit	Source
gf	-306.35	kJ/mol	Joback Method
hf	-743.78	kJ/mol	Joback Method
hfus	44.78	kJ/mol	Joback Method
hvap	89.71	kJ/mol	Joback Method
log10ws	-3.88		Crippen Method
logp	2.392		Crippen Method
mcvol	267.150	ml/mol	McGowan Method
pc	1660.55	kPa	Joback Method
rinpol	2378.00		NIST Webbook
rinpol	2378.00		NIST Webbook
tb	899.08	K	Joback Method
tc	1111.95	K	Joback Method
tf	563.47	K	Joback Method
vc	1.018	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	833.70	J/mol×K	899.08	Joback Method
cpg	846.82	J/mol×K	934.56	Joback Method
cpg	858.74	J/mol×K	970.04	Joback Method
cpg	869.48	J/mol×K	1005.51	Joback Method
cpg	879.05	J/mol×K	1040.99	Joback Method
cpg	887.49	J/mol×K	1076.47	Joback Method
cpg	894.80	J/mol×K	1111.95	Joback Method

Sources

Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
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=U308818&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume