L-Tyrosine, N,O-di(trifluoroacetyl)-, 2,2,3,3,3-pentafluoropropyl ester

Inchi: InChI=1S/C16H10F11NO5/c17-13(18,16(25,26)27)6-32-10(29)9(28-11(30)14(19,20)21)5

InchiKey: JGIISNXXOOYZIL-UHFFFAOYSA-N

Formula: C16H10F11NO5

SMILES: O=C(OCC(F)(F)C(F)(F)F)C(Cc1ccc(OC(=O)C(F)(F)F)cc1)NC(=O)C(F)(F)F

Mol. weight [g/mol]: 505.24

Physical Properties

Property code	Value	Unit	Source
gf	-2454.74	kJ/mol	Joback Method
hf	-2894.71	kJ/mol	Joback Method
hfus	43.82	kJ/mol	Joback Method
hvap	71.08	kJ/mol	Joback Method
log10ws	-5.34		Crippen Method
logp	3.485		Crippen Method
mcvol	258.440	ml/mol	McGowan Method
pc	1391.25	kPa	Joback Method
rinpol	1506.40		NIST Webbook
rinpol	1506.40		NIST Webbook
tb	832.37	K	Joback Method
tc	1021.15	K	Joback Method
tf	557.10	K	Joback Method
vc	1.060	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	807.24	J/mol×K	832.37	Joback Method
cpg	816.53	J/mol×K	863.83	Joback Method
cpg	825.01	J/mol×K	895.30	Joback Method
cpg	832.76	J/mol×K	926.76	Joback Method
cpg	839.84	J/mol×K	958.22	Joback Method
cpg	846.34	J/mol×K	989.68	Joback Method
cpg	852.32	J/mol×K	1021.15	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=U352341&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