tyrosine, trifluoroacetyl-isopropyl ester

Inchi: InChI=1S/C16H15F6NO5/c1-8(2)27-12(24)11(23-13(25)15(17,18)19)7-9-3-5-10(6-4-9)28
InchiKey: ROGJAPSCFDYSFC-UHFFFAOYSA-N
Formula: C16H15F6NO5
SMILES: CC(C)OC(=O)C(Cc1ccc(OC(=O)C(F)(F)F)cc1)NC(=O)C(F)(F)F
Mol. weight [g/mol]: 415.28

Physical Properties

Property code	Value	Unit	Source
gf	-1488.81	kJ/mol	Joback Method
hf	-1901.94	kJ/mol	Joback Method
hfus	39.73	kJ/mol	Joback Method
hvap	77.37	kJ/mol	Joback Method
log10ws	-4.48		Crippen Method
logp	2.695		Crippen Method
mcvol	249.590	ml/mol	McGowan Method
pc	1618.07	kPa	Joback Method
rinpol	1693.00		NIST Webbook
tb	842.04	K	Joback Method
tc	1039.90	K	Joback Method
tf	534.31	K	Joback Method
vc	0.987	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	767.09	J/mol×K	842.04	Joback Method
cpg	777.84	J/mol×K	875.02	Joback Method
cpg	787.67	J/mol×K	907.99	Joback Method
cpg	796.62	J/mol×K	940.97	Joback Method
cpg	804.74	J/mol×K	973.95	Joback Method
cpg	812.08	J/mol×K	1006.92	Joback Method
cpg	818.70	J/mol×K	1039.90	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=R268029&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