

Asparagine-threonine, N(«alpha»,«epsilon»)-trifluoroacetyl-N-O-permeth derivative

InChI: InChI=1S/C16H26F3N3O6/c1-9(27-6)12(14(25)28-7)22(5)13(24)10(8-11(23)20(2)3)21(4)
InChIKey: GNOCYVMVJWPDJH-UHFFFAOYSA-N

Formula: C16H26F3N3O6

SMILES: COC(=O)C(C(C)OC)N(C)C(=O)C(CC(=O)N(C)C)N(C)C(=O)C(F)(F)F

Mol. weight [g/mol]: 413.39

Physical Properties

Property code	Value	Unit	Source
gf	-898.41	kJ/mol	Joback Method
hf	-1498.66	kJ/mol	Joback Method
hfus	46.29	kJ/mol	Joback Method
hvap	84.23	kJ/mol	Joback Method
log10ws	-0.50		Crippen Method
logp	-0.111		Crippen Method
mcvol	289.570	ml/mol	McGowan Method
pc	1441.35	kPa	Joback Method
rinpol	2200.00		NIST Webbook
rinpol	2131.00		NIST Webbook
rinpol	2131.00		NIST Webbook
tb	856.38	K	Joback Method
tc	1050.45	K	Joback Method
tf	570.86	K	Joback Method
vc	1.071	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	924.06	J/molxK	856.38	Joback Method
cpg	937.53	J/molxK	888.72	Joback Method
cpg	949.97	J/molxK	921.07	Joback Method
cpg	961.41	J/molxK	953.41	Joback Method
cpg	971.91	J/molxK	985.76	Joback Method
cpg	981.50	J/molxK	1018.10	Joback Method
cpg	990.25	J/molxK	1050.45	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=R248723&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
rinpola:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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