L-Aspartic acid, N-(trifluoroacetyl)-, dibutyl ester

Other names: Aspartic acid, N-(trifluoroacetyl)-, dibutyl ester, L-
Asp, dibutyl ester, N-TFA
Asp, butyl ester, TFA

Inchi: InChI=1S/C14H22F3NO5/c1-3-5-7-22-11(19)9-10(12(20)23-8-6-4-2)18-13(21)14(15,16)1

InchiKey: AAAZDZBQEOVDCB-UHFFFAOYSA-N

Formula: C14H22F3NO5

SMILES: CCCCOC(=O)CC(NC(=O)C(F)(F)F)C(=O)OCCCC

Mol. weight [g/mol]: 341.32

CAS: 2926-77-4

Physical Properties

Property code	Value	Unit	Source
gf	-1024.40	kJ/mol	Joback Method
hf	-1483.36	kJ/mol	Joback Method
hfus	42.59	kJ/mol	Joback Method
hvap	74.12	kJ/mol	Joback Method
log10ws	-3.15		Crippen Method
logp	2.110		Crippen Method
mcvol	239.860	ml/mol	McGowan Method
pc	1597.44	kPa	Joback Method
rinpol	1676.00		NIST Webbook
tb	770.48	K	Joback Method
tc	952.42	K	Joback Method
tf	483.64	K	Joback Method
vc	0.946	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	726.04	J/mol×K	770.48	Joback Method
cpg	739.17	J/mol×K	800.80	Joback Method
cpg	751.48	J/mol×K	831.13	Joback Method
cpg	762.98	J/mol×K	861.45	Joback Method
cpg	773.69	J/mol×K	891.77	Joback Method

cpg	783.62	J/mol×K	922.09	Joback Method
cpg	792.81	J/mol×K	952.42	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=C2926774&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
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume