

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

Other names: Glutamic acid, N-(trifluoroacetyl)-, dibutyl ester, L-Glu, butyl ester, TFA
Glu TFA Bu

Inchi: InChI=1S/C15H24F3NO5/c1-3-5-9-23-12(20)8-7-11(13(21)24-10-6-4-2)19-14(22)15(16,1

InchiKey: YVLATHFLIIDMDU-LLVKDONJSA-N

Formula: C15H24F3NO5

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

Mol. weight [g/mol]: 355.35

CAS: 816-59-1

Physical Properties

Property code	Value	Unit	Source
gf	-1015.98	kJ/mol	Joback Method
hf	-1504.00	kJ/mol	Joback Method
hfus	45.18	kJ/mol	Joback Method
hvap	76.34	kJ/mol	Joback Method
log10ws	-3.57		Crippen Method
logp	2.500		Crippen Method
mcvol	253.950	ml/mol	McGowan Method
pc	1481.57	kPa	Joback Method
rinpol	1807.00		NIST Webbook
tb	793.36	K	Joback Method
tc	977.09	K	Joback Method
tf	494.91	K	Joback Method
vc	1.002	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	782.19	J/molxK	793.36	Joback Method
cpg	795.75	J/molxK	823.98	Joback Method
cpg	808.43	J/molxK	854.60	Joback Method
cpg	820.25	J/molxK	885.22	Joback Method
cpg	831.25	J/molxK	915.85	Joback Method

cpg	841.43	J/mol×K	946.47	Joback Method
cpg	850.83	J/mol×K	977.09	Joback Method

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
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=C816591&Units=SI

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
hvac:	Enthalpy of vaporization at standard conditions
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mccvol:	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

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