

DL-Alanyl-DL-alanyl-DL-alanine, N,N',N''-trimethyl-N''-(but-3-yn-1-yloxy-carbonyl)-, but-3-yn-1-yl ester

InChI: JChI=1S/C21H31N3O6/c1-9-11-13-29-20(27)17(5)23(7)18(25)15(3)22(6)19(26)16(4)24
InChIKey: JQKXJQPVSBRWOS-UHFFFAOYSA-N
Formula: C21H31N3O6
SMILES: C#CCCCOC(=O)C(C)N(C)C(=O)C(C)N(C)C(=O)C(C)N(C)C(=O)OCCC#C
Mol. weight [g/mol]: 421.49

Physical Properties

Property code	Value	Unit	Source
gf	171.42	kJ/mol	Joback Method
hf	-420.98	kJ/mol	Joback Method
hfus	63.36	kJ/mol	Joback Method
hvap	98.82	kJ/mol	Joback Method
log10ws	-2.50		Crippen Method
logp	0.727		Crippen Method
mvol	337.510	ml/mol	McGowan Method
pc	1369.71	kPa	Joback Method
rinpol	2656.00		NIST Webbook
rinpol	2656.00		NIST Webbook
tb	956.44	K	Joback Method
tc	1172.03	K	Joback Method
tf	716.96	K	Joback Method
vc	1.232	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1079.56	J/molxK	956.44	Joback Method
cpg	1093.37	J/molxK	992.37	Joback Method
cpg	1106.03	J/molxK	1028.30	Joback Method
cpg	1117.61	J/molxK	1064.23	Joback Method
cpg	1128.17	J/molxK	1100.17	Joback Method
cpg	1137.78	J/molxK	1136.10	Joback Method
cpg	1146.51	J/molxK	1172.03	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U392715&Units=SI
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

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
hvp:	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
rinp:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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