

Lysine, N,N-di(trifluoroacetyl)-, n-butyl ester

Other names:	Lys, butyl ester, TFA
Inchi:	InChI=1S/C14H20F6N2O4/c1-2-3-8-26-10(23)9(22-12(25)14(18,19)20)6-4-5-7-21-11(24)
InchiKey:	TYLLSQHVLXVPTR-SECBINFHSA-N
Formula:	C14H20F6N2O4
SMILES:	CCCCOC(=O)C(CCCNC(=O)C(F)(F)F)NC(=O)C(F)(F)F
Mol. weight [g/mol]:	394.31
CAS:	2926-74-1

Physical Properties

Property code	Value	Unit	Source
gf	-1411.60	kJ/mol	Joback Method
hf	-1894.75	kJ/mol	Joback Method
hfus	48.33	kJ/mol	Joback Method
hvap	74.40	kJ/mol	Joback Method
log10ws	-3.91		Crippen Method
logp	2.226		Crippen Method
mcvol	249.280	ml/mol	McGowan Method
pc	1493.04	kPa	Joback Method
rinpol	1811.00		NIST Webbook
rinpol	1811.00		NIST Webbook
tb	792.81	K	Joback Method
tc	973.59	K	Joback Method
tf	518.26	K	Joback Method
vc	1.006	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	778.70	J/molxK	792.81	Joback Method
cpg	790.76	J/molxK	822.94	Joback Method
cpg	802.02	J/molxK	853.07	Joback Method
cpg	812.51	J/molxK	883.20	Joback Method
cpg	822.29	J/molxK	913.33	Joback Method
cpg	831.40	J/molxK	943.46	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C2926741&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.cheméo.com/doc/models/crippen_log10ws
Joback Method:	https://en.wikipedia.org/wiki/Joback_method

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

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