

1-[4-(2,2,2-Trifluoroacetoxy)phenyl]-2-[(trifluoroacetoxy)amino]ethane

Other names:	n-Octonamine, TFA
Inchi:	InChI=1S/C14H8F9NO5/c15-12(16,17)9(25)24-5-8(29-11(27)14(21,22)23)6-1-3-7(4-2-6)
InchiKey:	AOQZMQBDUJCRTH-UHFFFAOYSA-N
Formula:	C14H8F9NO5
SMILES:	O=C(NCC(OC(=O)C(F)(F)F)c1ccc(OC(=O)C(F)(F)F)cc1)C(F)(F)F
Mol. weight [g/mol]:	441.20

Physical Properties

Property code	Value	Unit	Source
gf	-2084.80	kJ/mol	Joback Method
hf	-2452.46	kJ/mol	Joback Method
hfus	39.90	kJ/mol	Joback Method
hvap	69.56	kJ/mol	Joback Method
log10ws	-4.54		Crippen Method
logp	2.979		Crippen Method
mcvol	226.720	ml/mol	McGowan Method
pc	1710.36	kPa	Joback Method
rinpol	1450.00		NIST Webbook
rinpol	1487.00		NIST Webbook
rinpol	1497.00		NIST Webbook
rinpol	1487.00		NIST Webbook
rinpol	1497.00		NIST Webbook
rinpol	1450.00		NIST Webbook
tb	791.30	K	Joback Method
tc	978.20	K	Joback Method
tf	530.96	K	Joback Method
vc	0.923	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	682.59	J/molxK	791.30	Joback Method
cpg	691.62	J/molxK	822.45	Joback Method
cpg	699.87	J/molxK	853.60	Joback Method

cpg	707.37	J/mol×K	884.75	Joback Method
cpg	714.18	J/mol×K	915.90	Joback Method
cpg	720.36	J/mol×K	947.05	Joback Method
cpg	725.96	J/mol×K	978.20	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=U373479&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
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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