N-Trifluoroacetyl-2,5-dimethoxy-4-trifluoroacetoxy

Inchi: InChI=1S/C17H19F6NO5S/c1-27-11-9-13(30-7-3-6-29-15(26)17(21,22)23)12(28-2)8-10(
InchiKey: MNNNEXZALGRRBS-UHFFFAOYSA-N
Formula: C17H19F6NO5S
SMILES: COc1cc(SCCCOC(=O)C(F)(F)F)c(OC)cc1CCNC(=O)C(F)(F)F
Mol. weight [g/mol]: 463.39

Physical Properties

Property code	Value	Unit	Source
gf	-1437.73	kJ/mol	Joback Method
hf	-1912.73	kJ/mol	Joback Method
hfus	52.30	kJ/mol	Joback Method
hvap	84.18	kJ/mol	Joback Method
log10ws	-4.92		Crippen Method
logp	3.513		Crippen Method
mcvol	284.330	ml/mol	McGowan Method
pc	1380.93	kPa	Joback Method
rinpol	2105.00		NIST Webbook
rinpol	2105.00		NIST Webbook
tb	913.09	K	Joback Method
tc	1119.90	K	Joback Method
tf	607.32	K	Joback Method
vc	1.121	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	886.25	J/mol×K	913.09	Joback Method
cpg	896.95	J/mol×K	947.56	Joback Method
cpg	906.54	J/mol×K	982.03	Joback Method
cpg	915.04	J/mol×K	1016.50	Joback Method
cpg	922.48	J/mol×K	1050.96	Joback Method
cpg	928.88	J/mol×K	1085.43	Joback Method
cpg	934.29	J/mol×K	1119.90	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=R522813&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