

D-Erythronic acid «gamma»-lactone, bis(trifluoroacetate)

Inchi:	InChI=1S/C8H4F6O6/c9-7(10,11)5(16)19-2-1-18-4(15)3(2)20-6(17)8(12,13)14/h2-3H,1H
InchiKey:	DCRPKNGHHIPNOC-UHFFFAOYSA-N
Formula:	C8H4F6O6
SMILES:	O=C1OCC(OC(=O)C(F)(F)F)C1OC(=O)C(F)(F)F
Mol. weight [g/mol]:	310.10

Physical Properties

Property code	Value	Unit	Source
gf	-1794.41	kJ/mol	Joback Method
hf	-2121.77	kJ/mol	Joback Method
hfus	28.20	kJ/mol	Joback Method
hvap	52.92	kJ/mol	Joback Method
log10ws	-1.20		Crippen Method
logp	0.491		Crippen Method
mcvol	145.660	ml/mol	McGowan Method
pc	2621.78	kPa	Joback Method
tb	629.56	K	Joback Method
tc	819.45	K	Joback Method
tf	434.07	K	Joback Method
vc	0.586	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	419.59	J/molxK	629.56	Joback Method
cpg	430.36	J/molxK	661.21	Joback Method
cpg	440.39	J/molxK	692.86	Joback Method
cpg	449.71	J/molxK	724.50	Joback Method
cpg	458.31	J/molxK	756.15	Joback Method
cpg	466.20	J/molxK	787.80	Joback Method
cpg	473.39	J/molxK	819.45	Joback Method

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307I
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=U380214&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
mccvol:	McGowan's characteristic volume
pc:	Critical Pressure
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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