(S)-(-)-1,2,4-Butanetriol, 2,4-di(trifluoroacetate)

Inchi: InChI=1S/C8H8F6O5/c9-7(10,11)5(16)18-2-1-4(3-15)19-6(17)8(12,13)14/h4,15H,1-3H2
InchiKey: SFPBHDIELIHYRT-UHFFFAOYSA-N
Formula: C8H8F6O5
SMILES: O=C(OCCC(CO)OC(=O)C(F)(F)F)C(F)(F)F
Mol. weight [g/mol]: 298.14

Physical Properties

Property code	Value	Unit	Source
gf	-1753.80	kJ/mol	Joback Method
hf	-2049.72	kJ/mol	Joback Method
hfus	26.27	kJ/mol	Joback Method
hvap	60.51	kJ/mol	Joback Method
log10ws	-1.60		Crippen Method
logp	0.948		Crippen Method
mcvol	154.950	ml/mol	McGowan Method
pc	2436.25	kPa	Joback Method
rinpol	1046.00		NIST Webbook
rinpol	1046.00		NIST Webbook
tb	615.92	K	Joback Method
tc	774.18	K	Joback Method
tf	378.44	K	Joback Method
vc	0.630	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	429.12	J/mol×K	615.92	Joback Method
cpg	437.66	J/mol×K	642.30	Joback Method
cpg	445.72	J/mol×K	668.67	Joback Method
cpg	453.29	J/mol×K	695.05	Joback Method
cpg	460.41	J/mol×K	721.43	Joback Method
cpg	467.09	J/mol×K	747.80	Joback Method
cpg	473.34	J/mol×K	774.18	Joback Method

Sources

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=U374869&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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