1,2-Propanediol, bis(trifluoroacetate)

Inchi: InChI=1S/C7H6F6O4/c1-3(17-5(15)7(11,12)13)2-16-4(14)6(8,9)10/h3H,2H2,1H3
InchiKey: SRUSTRDCGNYRRA-UHFFFAOYSA-N
Formula: C7H6F6O4
SMILES: CC(COC(=O)C(F)(F)F)OC(=O)C(F)(F)F
Mol. weight [g/mol]: 268.11
CAS: 7556-83-4

Physical Properties

Property code	Value	Unit	Source
gf	-1625.40	kJ/mol	Joback Method
hf	-1876.85	kJ/mol	Joback Method
hfus	19.59	kJ/mol	Joback Method
hvap	41.61	kJ/mol	Joback Method
log10ws	-1.91		Crippen Method
logp	1.586		Crippen Method
mcvol	134.990	ml/mol	McGowan Method
pc	2445.89	kPa	Joback Method
rinpol	815.00		NIST Webbook
rinpol	815.00		NIST Webbook
tb	500.86	K	Joback Method
tc	661.19	K	Joback Method
tf	306.35	K	Joback Method
vc	0.555	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	335.30	J/mol×K	500.86	Joback Method
cpg	344.72	J/mol×K	527.58	Joback Method
cpg	353.65	J/mol×K	554.30	Joback Method
cpg	362.09	J/mol×K	581.02	Joback Method
cpg	370.05	J/mol×K	607.75	Joback Method
cpg	377.56	J/mol×K	634.47	Joback Method
cpg	384.62	J/mol×K	661.19	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C7556834&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
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

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