1,4:3,6-dianhydro-5-deoxy-2-O-(2,2,3,3,3-pentaflu

Inchi: InChI=1S/C9H7F5O4/c10-8(11,9(12,13)14)7(15)18-5-3-17-4-1-2-16-6(4)5/h1-2,4-6H,3H2
InchiKey: WKHAWIGEKZJLAK-UHFFFAOYSA-N
Formula: C9H7F5O4
SMILES: O=C(OC1COC2C=COC21)C(F)(F)C(F)(F)F
Mol. weight [g/mol]: 274.14

Physical Properties

Property code	Value	Unit	Source
gf	-1230.08	kJ/mol	Joback Method
hf	-1565.22	kJ/mol	Joback Method
hfus	32.75	kJ/mol	Joback Method
hvap	47.28	kJ/mol	Joback Method
log10ws	-2.08		Crippen Method
logp	1.407		Crippen Method
mcvol	139.680	ml/mol	McGowan Method
pc	2690.21	kPa	Joback Method
rinpol	1252.00		NIST Webbook
rinpol	1252.00		NIST Webbook
tb	541.91	K	Joback Method
tc	731.80	K	Joback Method
tf	349.64	K	Joback Method
vc	0.556	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	386.53	J/mol×K	541.91	Joback Method
cpg	399.92	J/mol×K	573.56	Joback Method
cpg	412.32	J/mol×K	605.21	Joback Method
cpg	423.78	J/mol×K	636.85	Joback Method
cpg	434.37	J/mol×K	668.50	Joback Method
cpg	444.14	J/mol×K	700.15	Joback Method
cpg	453.15	J/mol×K	731.80	Joback Method

Sources

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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U375751&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
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume