

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

Inchi:	InChI=1S/C10H7F7O4/c11-8(12,9(13,14)10(15,16)17)7(18)21-5-3-20-4-1-2-19-6(4)5/h1-
InchiKey:	YFTFQQPXTUVRGZ-UHFFFAOYSA-N
Formula:	C10H7F7O4
SMILES:	O=C(OC1COC2C=COC21)C(F)(F)C(F)(F)C(F)(F)F
Mol. weight [g/mol]:	324.15

Physical Properties

Property code	Value	Unit	Source
gf	-1608.44	kJ/mol	Joback Method
hf	-1986.83	kJ/mol	Joback Method
hfus	34.08	kJ/mol	Joback Method
hvap	46.58	kJ/mol	Joback Method
log10ws	-2.81		Crippen Method
logp	2.042		Crippen Method
mcvol	157.310	ml/mol	McGowan Method
pc	2278.41	kPa	Joback Method
rinsol	1320.00		NIST Webbook
tb	560.10	K	Joback Method
tc	741.22	K	Joback Method
tf	364.51	K	Joback Method
vc	0.637	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	453.48	J/molxK	560.10	Joback Method
cpg	466.95	J/molxK	590.29	Joback Method
cpg	479.39	J/molxK	620.47	Joback Method
cpg	490.85	J/molxK	650.66	Joback Method
cpg	501.40	J/molxK	680.84	Joback Method
cpg	511.10	J/molxK	711.03	Joback Method
cpg	520.03	J/molxK	741.22	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=U375750&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
h vap:	Enthalpy of vaporization at standard conditions
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
m cvol:	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

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