Zearalenone, bis(pentafluoropropionate)

Other names: (E)-3-Methyl-1,7-dioxo-3,4,5,6,7,8,9,10-octahydro-1H-benzo[c][1]oxacyclotetradecine-14, 17924-92-4, F5P bis(2,2,3,3,3-pentafluoropropanoate)

Inchi: InChI=1S/C24H20F10O7/c1-12-6-5-9-14(35)8-4-2-3-7-13-10-15(40-19(37)21(25,26)23(2

InchiKey: SSGUZRJHMCNOEF-XVNBXDOJSA-N

Formula: C24H20F10O7

SMILES: CC1CCCC(=O)CCCC=Cc2cc(OC(=O)C(F)(F)C(F)(F)F)cc(OC(=O)C(F)(F)C(F)(F)F)c2C(=

Mol. weight [g/mol]: 610.40

CAS: 35-28-9

Physical Properties

Property code	Value	Unit	Source
gf	-2519.35	kJ/mol	Joback Method
hf	-3154.53	kJ/mol	Joback Method
hfus	44.96	kJ/mol	Joback Method
hvap	93.00	kJ/mol	Joback Method
log10ws	-8.59		Crippen Method
logp	6.374		Crippen Method
mcvol	351.690	ml/mol	McGowan Method
pc	1063.79	kPa	Joback Method
rinpol	2376.00		NIST Webbook
rinpol	2376.00		NIST Webbook
tb	1129.42	K	Joback Method
tc	1382.83	K	Joback Method
tf	734.15	K	Joback Method
vc	1.361	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1224.61	J/mol×K	1129.42	Joback Method
cpg	1225.21	J/mol×K	1171.65	Joback Method
cpg	1222.79	J/mol×K	1213.89	Joback Method
cpg	1217.37	J/mol×K	1256.12	Joback Method
cpg	1208.95	J/mol×K	1298.36	Joback Method

cpg	1197.56	J/mol×K	1340.59	Joback Method
cpg	1183.22	J/mol×K	1382.83	Joback Method

Sources

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=C35289&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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