Ketogluconic acid methyl ester, tetrakis(trifluoroacetate) (isomer 3)

Inchi: InChI=1S/C15H8F12O11/c1-34-7(29)4(28)6(38-11(33)15(25,26)27)5(37-10(32)14(22,23)
InchiKey: ODXLNIXRVBTRPN-UHFFFAOYSA-N
Formula: C15H8F12O11
SMILES: COC(=O)C(=O)C(OC(=O)C(F)(F)F)C(OC(=O)C(F)(F)F)C(COC(=O)C(F)(F)F)OC(=O)C(F
Mol. weight [g/mol]: 592.20

Physical Properties

Property code	Value	Unit	Source
gf	-3556.78	kJ/mol	Joback Method
hf	-4093.67	kJ/mol	Joback Method
hfus	46.87	kJ/mol	Joback Method
hvap	85.36	kJ/mol	Joback Method
log10ws	-2.68		Crippen Method
logp	1.256		Crippen Method
mcvol	282.220	ml/mol	McGowan Method
pc	1270.97	kPa	Joback Method
rinpol	1236.80		NIST Webbook
tb	954.92	K	Joback Method
tc	1176.49	K	Joback Method
tf	641.30	K	Joback Method
vc	1.155	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	904.59	J/mol×K	954.92	Joback Method
cpg	910.91	J/mol×K	991.85	Joback Method
cpg	916.02	J/mol×K	1028.78	Joback Method
cpg	919.96	J/mol×K	1065.71	Joback Method
cpg	922.81	J/mol×K	1102.64	Joback Method
cpg	924.61	J/mol×K	1139.57	Joback Method
cpg	925.43	J/mol×K	1176.49	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U380315&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