Glutaric acid, di(1-(pentafluorophenyl)ethyl) ester

Inchi: InChI=1S/C21H14F10O4/c1-6(10-12(22)16(26)20(30)17(27)13(10)23)34-8(32)4-3-5-9(33

InchiKey: ZFMGVFJYTDULDB-UHFFFAOYSA-N

Formula: C21H14F10O4

SMILES: CC(OC(=O)CCCC(=O)OC(C)c1c(F)c(F)c(F)c(F)c1F)c1c(F)c(F)c(F)c(F)c1F

Mol. weight [g/mol]: 520.32

Physical Properties

Property code	Value	Unit	Source
gf	-2166.36	kJ/mol	Joback Method
hf	-2579.67	kJ/mol	Joback Method
hfus	63.67	kJ/mol	Joback Method
hvap	82.88	kJ/mol	Joback Method
log10ws	-8.78		Crippen Method
logp	6.157		Crippen Method
mcvol	291.810	ml/mol	McGowan Method
pc	1065.18	kPa	Joback Method
rinpol	2206.00		NIST Webbook
rinpol	2206.00		NIST Webbook
tb	927.44	K	Joback Method
tc	1136.49	K	Joback Method
tf	624.69	K	Joback Method
vc	1.212	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	900.94	J/mol×K	927.44	Joback Method
cpg	911.78	J/mol×K	962.28	Joback Method
cpg	921.37	J/mol×K	997.12	Joback Method
cpg	929.70	J/mol×K	1031.97	Joback Method
cpg	936.77	J/mol×K	1066.81	Joback Method
cpg	942.57	J/mol×K	1101.65	Joback Method
cpg	947.09	J/mol×K	1136.49	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=U377014&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