Glutaric acid, ethyl 1-(pentafluorophenyl)ethyl ester

Inchi: InChI=1S/C15H15F5O4/c1-3-23-8(21)5-4-6-9(22)24-7(2)10-11(16)13(18)15(20)14(19)12

InchiKey: UGJUTYGNPIPJOY-UHFFFAOYSA-N

Formula: C15H15F5O4

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

Mol. weight [g/mol]: 354.27

Physical Properties

Property code	Value	Unit	Source
gf	-1304.65	kJ/mol	Joback Method
hf	-1649.18	kJ/mol	Joback Method
hfus	44.15	kJ/mol	Joback Method
hvap	68.41	kJ/mol	Joback Method
log10ws	-5.05		Crippen Method
logp	3.720		Crippen Method
mcvol	222.180	ml/mol	McGowan Method
pc	1565.99	kPa	Joback Method
rinpol	1747.00		NIST Webbook
rinpol	1747.00		NIST Webbook
tb	742.67	K	Joback Method
tc	923.26	K	Joback Method
tf	480.10	K	Joback Method
vc	0.899	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	629.44	J/mol×K	742.67	Joback Method
cpg	641.60	J/mol×K	772.77	Joback Method
cpg	653.07	J/mol×K	802.87	Joback Method
cpg	663.82	J/mol×K	832.97	Joback Method
cpg	673.86	J/mol×K	863.07	Joback Method
cpg	683.18	J/mol×K	893.16	Joback Method
cpg	691.78	J/mol×K	923.26	Joback Method

Sources

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=U376994&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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