Glutaric acid, ethyl 2-(pentafluorophenoxy)ethyl ester

Inchi: InChI=1S/C15H15F5O5/c1-2-23-8(21)4-3-5-9(22)24-6-7-25-15-13(19)11(17)10(16)12(18

InchiKey: PIUAGSQUUGBERS-UHFFFAOYSA-N

Formula: C15H15F5O5

SMILES: CCOC(=O)CCCC(=O)OCCOc1c(F)c(F)c(F)c(F)c1F

Mol. weight [g/mol]: 370.27

Physical Properties

Property code	Value	Unit	Source
gf	-1407.21	kJ/mol	Joback Method
hf	-1776.12	kJ/mol	Joback Method
hfus	48.86	kJ/mol	Joback Method
hvap	71.21	kJ/mol	Joback Method
log10ws	-4.32		Crippen Method
logp	3.037		Crippen Method
mcvol	228.050	ml/mol	McGowan Method
pc	1535.46	kPa	Joback Method
rinpol	1965.00		NIST Webbook
tb	765.53	K	Joback Method
tc	946.05	K	Joback Method
tf	517.33	K	Joback Method
vc	0.923	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	655.57	J/mol×K	765.53	Joback Method
cpg	667.50	J/mol×K	795.62	Joback Method
cpg	678.69	J/mol×K	825.70	Joback Method
cpg	689.13	J/mol×K	855.79	Joback Method
cpg	698.81	J/mol×K	885.88	Joback Method
cpg	707.72	J/mol×K	915.96	Joback Method
cpg	715.83	J/mol×K	946.05	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=U377320&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