Glutaric acid, isobutyl 2-(pentafluorophenoxy)ethyl ester

Inchi: InChI=1S/C17H19F5O5/c1-9(2)8-27-11(24)5-3-4-10(23)25-6-7-26-17-15(21)13(19)12(18
InchiKey: UEAVWPLUALMFRS-UHFFFAOYSA-N
Formula: C17H19F5O5
SMILES: CC(C)COC(=O)CCCC(=O)OCCOc1c(F)c(F)c(F)c(F)c1F
Mol. weight [g/mol]: 398.32

Physical Properties

Property code	Value	Unit	Source
gf	-1392.81	kJ/mol	Joback Method
hf	-1822.68	kJ/mol	Joback Method
hfus	50.52	kJ/mol	Joback Method
hvap	75.27	kJ/mol	Joback Method
log10ws	-4.92		Crippen Method
logp	3.674		Crippen Method
mcvol	256.230	ml/mol	McGowan Method
pc	1335.88	kPa	Joback Method
rinpol	2117.00		NIST Webbook
rinpol	2117.00		NIST Webbook
tb	810.85	K	Joback Method
tc	996.64	K	Joback Method
tf	524.87	K	Joback Method
vc	1.030	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	767.40	J/mol×K	810.85	Joback Method
cpg	780.34	J/mol×K	841.82	Joback Method
cpg	792.37	J/mol×K	872.78	Joback Method
cpg	803.48	J/mol×K	903.75	Joback Method
cpg	813.67	J/mol×K	934.71	Joback Method
cpg	822.93	J/mol×K	965.68	Joback Method
cpg	831.23	J/mol×K	996.64	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=U377322&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