Glutaric acid, 2-(pentafluorophenoxy)ethyl pentyl ester

Inchi: InChI=1S/C18H21F5O5/c1-2-3-4-8-26-11(24)6-5-7-12(25)27-9-10-28-18-16(22)14(20)13

InchiKey: VKAUBUJETYPEOH-UHFFFAOYSA-N

Formula: C18H21F5O5

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

Mol. weight [g/mol]: 412.35

Physical Properties

Property code	Value	Unit	Source
gf	-1381.95	kJ/mol	Joback Method
hf	-1838.04	kJ/mol	Joback Method
hfus	56.63	kJ/mol	Joback Method
hvap	77.89	kJ/mol	Joback Method
log10ws	-5.58		Crippen Method
logp	4.208		Crippen Method
mcvol	270.320	ml/mol	McGowan Method
pc	1239.83	kPa	Joback Method
rinpol	2260.00		NIST Webbook
rinpol	2260.00		NIST Webbook
tb	834.17	K	Joback Method
tc	1022.43	K	Joback Method
tf	551.14	K	Joback Method
vc	1.091	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	823.88	J/mol×K	834.17	Joback Method
cpg	837.19	J/mol×K	865.55	Joback Method
cpg	849.54	J/mol×K	896.92	Joback Method
cpg	860.90	J/mol×K	928.30	Joback Method
cpg	871.27	J/mol×K	959.68	Joback Method
cpg	880.64	J/mol×K	991.05	Joback Method
cpg	889.00	J/mol×K	1022.43	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=U377324&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