Glutaric acid, 2,2,3,3,4,4,5,5-octafluoropentyl pentafluorobenzyl ester

Inchi: InChI=1S/C17H11F13O4/c18-9-6(10(19)12(21)13(22)11(9)20)4-33-7(31)2-1-3-8(32)34-5

InchiKey: LOPYOOLEBMINMX-UHFFFAOYSA-N

Formula: C17H11F13O4

SMILES: O=C(CCCC(=O)OCC(F)(F)C(F)(F)C(F)(F)C(F)(F)F)OCc1c(F)c(F)c(F)c(F)c1F

Mol. weight [g/mol]: 526.25

Physical Properties

Property code	Value	Unit	Source
gf	-2837.77	kJ/mol	Joback Method
hf	-3285.59	kJ/mol	Joback Method
hfus	51.73	kJ/mol	Joback Method
hvap	62.44	kJ/mol	Joback Method
log10ws	-7.18		Crippen Method
logp	5.310		Crippen Method
mcvol	264.520	ml/mol	McGowan Method
pc	1094.99	kPa	Joback Method
rinpol	1804.00		NIST Webbook
rinpol	1804.00		NIST Webbook
tb	772.90	K	Joback Method
tc	946.41	K	Joback Method
tf	514.62	K	Joback Method
vc	1.123	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	806.63	J/mol×K	772.90	Joback Method
cpg	817.68	J/mol×K	801.82	Joback Method
cpg	827.96	J/mol×K	830.74	Joback Method
cpg	837.50	J/mol×K	859.65	Joback Method
cpg	846.35	J/mol×K	888.57	Joback Method
cpg	854.53	J/mol×K	917.49	Joback Method
cpg	862.08	J/mol×K	946.41	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=U391926&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