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

Inchi: InChI=1S/C17H16F8O4/c1-10-5-2-3-6-11(10)29-13(27)8-4-7-12(26)28-9-15(20,21)17(24

InchiKey: RKGFSSLWUPNJOH-UHFFFAOYSA-N

Formula: C17H16F8O4

SMILES: Cc1ccccc1OC(=O)CCCC(=O)OCC(F)(F)C(F)(F)C(F)(F)C(F)F

Mol. weight [g/mol]: 436.29

Physical Properties

Property code	Value	Unit	Source
gf	-1825.20	kJ/mol	Joback Method
hf	-2259.16	kJ/mol	Joback Method
hfus	37.89	kJ/mol	Joback Method
hvap	63.87	kJ/mol	Joback Method
log10ws	-5.73		Crippen Method
logp	4.785		Crippen Method
mcvol	255.670	ml/mol	McGowan Method
pc	1334.91	kPa	Joback Method
rinpol	1903.00		NIST Webbook
rinpol	1903.00		NIST Webbook
tb	756.63	K	Joback Method
tc	937.01	K	Joback Method
tf	461.59	K	Joback Method
vc	1.032	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	772.30	J/mol×K	756.63	Joback Method
cpg	784.83	J/mol×K	786.69	Joback Method
cpg	796.47	J/mol×K	816.76	Joback Method
cpg	807.29	J/mol×K	846.82	Joback Method
cpg	817.32	J/mol×K	876.88	Joback Method
cpg	826.62	J/mol×K	906.95	Joback Method
cpg	835.24	J/mol×K	937.01	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U391803&Units=SI
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

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