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

Inchi: InChI=1S/C22H18F8O4/c23-19(24)21(27,28)22(29,30)20(25,26)13-33-17(31)7-4-8-18(32

InchiKey: VJNSVNVJOCWDCP-UHFFFAOYSA-N

Formula: C22H18F8O4

SMILES: O=C(CCCC(=O)Oc1ccc(-c2ccccc2)cc1)OCC(F)(F)C(F)(F)C(F)(F)C(F)F

Mol. weight [g/mol]: 498.36

Physical Properties

Property code	Value	Unit	Source
gf	-1670.69	kJ/mol	Joback Method
hf	-2125.83	kJ/mol	Joback Method
hfus	44.88	kJ/mol	Joback Method
hvap	77.28	kJ/mol	Joback Method
log10ws	-7.86		Crippen Method
logp	6.144		Crippen Method
mcvol	302.360	ml/mol	McGowan Method
pc	1200.62	kPa	Joback Method
rinpol	2581.00		NIST Webbook
rinpol	2581.00		NIST Webbook
tb	897.71	K	Joback Method
tc	1103.18	K	Joback Method
tf	544.36	K	Joback Method
vc	1.204	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	958.10	J/mol×K	897.71	Joback Method
cpg	969.98	J/mol×K	931.95	Joback Method
cpg	980.88	J/mol×K	966.20	Joback Method
cpg	990.91	J/mol×K	1000.44	Joback Method
cpg	1000.16	J/mol×K	1034.69	Joback Method
cpg	1008.74	J/mol×K	1068.93	Joback Method
cpg	1016.73	J/mol×K	1103.18	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U390118&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
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

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