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

Inchi: InChI=1S/C23H20F8O4/c24-20(25)22(28,29)23(30,31)21(26,27)14-34-17(32)12-7-13-18

InchiKey: QJAYBVNXPKKQQK-UHFFFAOYSA-N

Formula: C23H20F8O4

SMILES: O=C(CCCC(=O)OC(c1ccccc1)c1ccccc1)OCC(F)(F)C(F)(F)C(F)(F)C(F)F

Mol. weight [g/mol]: 512.39

Physical Properties

Property code	Value	Unit	Source
gf	-1655.08	kJ/mol	Joback Method
hf	-2140.28	kJ/mol	Joback Method
hfus	44.33	kJ/mol	Joback Method
hvap	78.46	kJ/mol	Joback Method
log10ws	-7.20		Crippen Method
logp	6.204		Crippen Method
mcvol	316.450	ml/mol	McGowan Method
pc	1142.12	kPa	Joback Method
rinpol	2428.00		NIST Webbook
rinpol	2428.00		NIST Webbook
tb	915.17	K	Joback Method
tc	1123.21	K	Joback Method
tf	528.11	K	Joback Method
vc	1.254	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1017.62	J/mol×K	915.17	Joback Method
cpg	1029.91	J/mol×K	949.84	Joback Method
cpg	1041.20	J/mol×K	984.52	Joback Method
cpg	1051.61	J/mol×K	1019.19	Joback Method
cpg	1061.25	J/mol×K	1053.86	Joback Method
cpg	1070.22	J/mol×K	1088.54	Joback Method
cpg	1078.64	J/mol×K	1123.21	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U393338&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