Glutaric acid, 2,2,3,3,4,4,5,5-octafluoropentyl 1-phenylpropyl ester

Inchi: InChI=1S/C19H20F8O4/c1-2-13(12-7-4-3-5-8-12)31-15(29)10-6-9-14(28)30-11-17(22,23)

InchiKey: WIDUQDKLWUVRTH-UHFFFAOYSA-N

Formula: C19H20F8O4

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

Mol. weight [g/mol]: 464.35

Physical Properties

Property code	Value	Unit	Source
gf	-1801.17	kJ/mol	Joback Method
hf	-2294.25	kJ/mol	Joback Method
hfus	39.93	kJ/mol	Joback Method
hvap	67.28	kJ/mol	Joback Method
log10ws	-6.32		Crippen Method
logp	5.565		Crippen Method
mcvol	283.850	ml/mol	McGowan Method
pc	1184.16	kPa	Joback Method
rinpol	1988.00		NIST Webbook
rinpol	1988.00		NIST Webbook
tb	796.97	K	Joback Method
tc	981.16	K	Joback Method
tf	456.61	K	Joback Method
vc	1.139	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	885.33	J/mol×K	796.97	Joback Method
cpg	898.76	J/mol×K	827.67	Joback Method
cpg	911.22	J/mol×K	858.37	Joback Method
cpg	922.79	J/mol×K	889.06	Joback Method
cpg	933.52	J/mol×K	919.76	Joback Method
cpg	943.49	J/mol×K	950.46	Joback Method
cpg	952.75	J/mol×K	981.16	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U392044&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