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

Inchi: InChI=1S/C16H9F13O4/c17-7-8(18)10(20)12(11(21)9(7)19)33-6(31)3-1-2-5(30)32-4-14(2

InchiKey: LMYSMQVKPSDHMA-UHFFFAOYSA-N

Formula: C16H9F13O4

SMILES: O=C(CCCC(=O)Oc1c(F)c(F)c(F)c(F)c1F)OCC(F)(F)C(F)(F)C(F)(F)C(F)F

Mol. weight [g/mol]: 512.22

Physical Properties

Property code	Value	Unit	Source
gf	-2846.19	kJ/mol	Joback Method
hf	-3264.95	kJ/mol	Joback Method
hfus	49.14	kJ/mol	Joback Method
hvap	60.21	kJ/mol	Joback Method
log10ws	-6.91		Crippen Method
logp	5.172		Crippen Method
mcvol	250.430	ml/mol	McGowan Method
pc	1168.02	kPa	Joback Method
rinpol	1660.00		NIST Webbook
rinpol	1660.00		NIST Webbook
tb	750.02	K	Joback Method
tc	919.30	K	Joback Method
tf	503.35	K	Joback Method
vc	1.067	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	752.55	J/mol×K	750.02	Joback Method
cpg	763.04	J/mol×K	778.23	Joback Method
cpg	772.81	J/mol×K	806.45	Joback Method
cpg	781.89	J/mol×K	834.66	Joback Method
cpg	790.31	J/mol×K	862.87	Joback Method
cpg	798.11	J/mol×K	891.08	Joback Method
cpg	805.32	J/mol×K	919.30	Joback Method

Sources

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=U392104&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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