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

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

InchiKey: OVCPXWXAXTVWQC-UHFFFAOYSA-N

Formula: C19H20F8O4

SMILES: CCCc1ccccc1OC(=O)CCCC(=O)OCC(F)(F)C(F)(F)C(F)(F)C(F)F

Mol. weight [g/mol]: 464.35

Physical Properties

Property code	Value	Unit	Source
gf	-1808.36	kJ/mol	Joback Method
hf	-2300.44	kJ/mol	Joback Method
hfus	43.07	kJ/mol	Joback Method
hvap	68.33	kJ/mol	Joback Method
log10ws	-6.47		Crippen Method
logp	5.429		Crippen Method
mcvol	283.850	ml/mol	McGowan Method
pc	1165.63	kPa	Joback Method
rinpol	2025.00		NIST Webbook
rinpol	2025.00		NIST Webbook
tb	802.39	K	Joback Method
tc	986.51	K	Joback Method
tf	484.13	K	Joback Method
vc	1.145	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	883.90	J/mol×K	802.39	Joback Method
cpg	897.16	J/mol×K	833.08	Joback Method
cpg	909.49	J/mol×K	863.76	Joback Method
cpg	920.95	J/mol×K	894.45	Joback Method
cpg	931.60	J/mol×K	925.14	Joback Method
cpg	941.49	J/mol×K	955.83	Joback Method
cpg	950.69	J/mol×K	986.51	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U392136&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