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

Inchi: InChI=1S/C17H14F8O5/c18-14(19)16(22,23)17(24,25)15(20,21)9-29-12(27)6-3-7-13(28)

InchiKey: JLYWIIMWFKQOPC-UHFFFAOYSA-N

Formula: C17H14F8O5

SMILES: O=Cc1ccccc1OC(=O)CCCC(=O)OCC(F)(F)C(F)(F)C(F)(F)C(F)F

Mol. weight [g/mol]: 450.28

Physical Properties

Property code	Value	Unit	Source
gf	-1924.72	kJ/mol	Joback Method
hf	-2344.74	kJ/mol	Joback Method
hfus	40.18	kJ/mol	Joback Method
hvap	70.59	kJ/mol	Joback Method
log10ws	-5.49		Crippen Method
logp	4.289		Crippen Method
mcvol	257.240	ml/mol	McGowan Method
pc	1410.13	kPa	Joback Method
rinpol	2112.00		NIST Webbook
rinpol	2112.00		NIST Webbook
tb	805.29	K	Joback Method
tc	992.32	K	Joback Method
tf	503.59	K	Joback Method
vc	1.050	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	786.43	J/mol×K	805.29	Joback Method
cpg	797.37	J/mol×K	836.46	Joback Method
cpg	807.47	J/mol×K	867.63	Joback Method
cpg	816.76	J/mol×K	898.81	Joback Method
cpg	825.31	J/mol×K	929.98	Joback Method
cpg	833.19	J/mol×K	961.15	Joback Method
cpg	840.44	J/mol×K	992.32	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U390246&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