Glutaric acid, 2-methylhex-3-yl 2,3,4,5-tetrafluorobenzyl ester

Inchi: InChI=1S/C19H24F4O4/c1-4-6-14(11(2)3)27-16(25)8-5-7-15(24)26-10-12-9-13(20)18(22

InchiKey: ZABYUAYNEIVWQO-UHFFFAOYSA-N

Formula: C19H24F4O4

SMILES: CCCC(OC(=O)CCCC(=O)OCc1cc(F)c(F)c(F)c1F)C(C)C

Mol. weight [g/mol]: 392.39

Physical Properties

Property code	Value	Unit	Source
gf	-1068.97	kJ/mol	Joback Method
hf	-1529.44	kJ/mol	Joback Method
hfus	48.30	kJ/mol	Joback Method
hvap	77.08	kJ/mol	Joback Method
log10ws	-6.30		Crippen Method
logp	4.824		Crippen Method
mcvol	276.770	ml/mol	McGowan Method
pc	1237.22	kPa	Joback Method
rinpol	2192.00		NIST Webbook
rinpol	2192.00		NIST Webbook
tb	829.50	K	Joback Method
tc	1020.08	K	Joback Method
tf	497.07	K	Joback Method
vc	1.099	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	847.73	J/mol×K	829.50	Joback Method
cpg	862.11	J/mol×K	861.26	Joback Method
cpg	875.49	J/mol×K	893.03	Joback Method
cpg	887.87	J/mol×K	924.79	Joback Method
cpg	899.27	J/mol×K	956.55	Joback Method
cpg	909.68	J/mol×K	988.32	Joback Method
cpg	919.12	J/mol×K	1020.08	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U377443&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