Glutaric acid, di(2,3,4,5-tetrafluorobenzyl) ester

Inchi: InChI=1S/C19H12F8O4/c20-10-4-8(14(22)18(26)16(10)24)6-30-12(28)2-1-3-13(29)31-7-

InchiKey: DWFQAPJOSPRJPH-UHFFFAOYSA-N

Formula: C19H12F8O4

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

Mol. weight [g/mol]: 456.28

Physical Properties

Property code	Value	Unit	Source
gf	-1769.44	kJ/mol	Joback Method
hf	-2112.67	kJ/mol	Joback Method
hfus	60.15	kJ/mol	Joback Method
hvap	79.51	kJ/mol	Joback Method
log10ws	-7.35		Crippen Method
logp	4.756		Crippen Method
mcvol	260.090	ml/mol	McGowan Method
pc	1305.17	kPa	Joback Method
rinpol	2365.00		NIST Webbook
rinpol	2365.00		NIST Webbook
tb	874.06	K	Joback Method
tc	1071.29	K	Joback Method
tf	605.93	K	Joback Method
vc	1.075	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	774.48	J/mol×K	874.06	Joback Method
cpg	785.08	J/mol×K	906.93	Joback Method
cpg	794.71	J/mol×K	939.80	Joback Method
cpg	803.35	J/mol×K	972.68	Joback Method
cpg	811.01	J/mol×K	1005.55	Joback Method
cpg	817.68	J/mol×K	1038.42	Joback Method
cpg	823.37	J/mol×K	1071.29	Joback Method

Sources

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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U377457&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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