Glutaric acid, pentyl 2,3,4,5-tetrafluorobenzyl ester

Inchi: InChI=1S/C17H20F4O4/c1-2-3-4-8-24-13(22)6-5-7-14(23)25-10-11-9-12(18)16(20)17(21

InchiKey: JFXFGZOXJRUOJK-UHFFFAOYSA-N

Formula: C17H20F4O4

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

Mol. weight [g/mol]: 364.33

Physical Properties

Property code	Value	Unit	Source
gf	-1080.93	kJ/mol	Joback Method
hf	-1477.60	kJ/mol	Joback Method
hfus	50.16	kJ/mol	Joback Method
hvap	73.40	kJ/mol	Joback Method
log10ws	-5.59		Crippen Method
logp	4.190		Crippen Method
mcvol	248.590	ml/mol	McGowan Method
pc	1405.90	kPa	Joback Method
rinpol	2134.00		NIST Webbook
rinpol	2134.00		NIST Webbook
tb	784.62	K	Joback Method
tc	968.87	K	Joback Method
tf	504.53	K	Joback Method
vc	1.000	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	732.41	J/mol×K	784.62	Joback Method
cpg	745.82	J/mol×K	815.33	Joback Method
cpg	758.41	J/mol×K	846.04	Joback Method
cpg	770.16	J/mol×K	876.74	Joback Method
cpg	781.08	J/mol×K	907.45	Joback Method
cpg	791.18	J/mol×K	938.16	Joback Method
cpg	800.45	J/mol×K	968.87	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U377442&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

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