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

Inchi: InChI=1S/C15H16F4O4/c1-2-6-22-11(20)4-3-5-12(21)23-8-9-7-10(16)14(18)15(19)13(9)1

InchiKey: HXVILTBIQCNCJD-UHFFFAOYSA-N

Formula: C15H16F4O4

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

Mol. weight [g/mol]: 336.28

Physical Properties

Property code	Value	Unit	Source
gf	-1097.77	kJ/mol	Joback Method
hf	-1436.32	kJ/mol	Joback Method
hfus	44.98	kJ/mol	Joback Method
hvap	68.95	kJ/mol	Joback Method
log10ws	-4.75		Crippen Method
logp	3.410		Crippen Method
mcvol	220.410	ml/mol	McGowan Method
pc	1632.49	kPa	Joback Method
rinpol	1933.00		NIST Webbook
rinpol	1933.00		NIST Webbook
tb	738.86	K	Joback Method
tc	921.17	K	Joback Method
tf	481.99	K	Joback Method
vc	0.887	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	622.10	J/mol×K	738.86	Joback Method
cpg	634.59	J/mol×K	769.24	Joback Method
cpg	646.36	J/mol×K	799.63	Joback Method
cpg	657.40	J/mol×K	830.01	Joback Method
cpg	667.73	J/mol×K	860.40	Joback Method
cpg	677.33	J/mol×K	890.78	Joback Method
cpg	686.21	J/mol×K	921.17	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U377439&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