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

Inchi: InChI=1S/C18H22F4O4/c1-2-3-4-5-9-25-14(23)7-6-8-15(24)26-11-12-10-13(19)17(21)18

InchiKey: XXKAYSDUBXRMMZ-UHFFFAOYSA-N

Formula: C18H22F4O4

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

Mol. weight [g/mol]: 378.36

Physical Properties

Property code	Value	Unit	Source
gf	-1072.51	kJ/mol	Joback Method
hf	-1498.24	kJ/mol	Joback Method
hfus	52.75	kJ/mol	Joback Method
hvap	75.63	kJ/mol	Joback Method
log10ws	-6.01		Crippen Method
logp	4.580		Crippen Method
mcvol	262.680	ml/mol	McGowan Method
pc	1309.90	kPa	Joback Method
rinpol	2240.00		NIST Webbook
rinpol	2240.00		NIST Webbook
tb	807.50	K	Joback Method
tc	993.68	K	Joback Method
tf	515.80	K	Joback Method
vc	1.056	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	789.08	J/mol×K	807.50	Joback Method
cpg	802.92	J/mol×K	838.53	Joback Method
cpg	815.87	J/mol×K	869.56	Joback Method
cpg	827.93	J/mol×K	900.59	Joback Method
cpg	839.10	J/mol×K	931.62	Joback Method
cpg	849.38	J/mol×K	962.65	Joback Method
cpg	858.79	J/mol×K	993.68	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U377444&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