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

Inchi: InChI=1S/C30H46F4O4/c1-2-3-4-5-6-7-8-9-10-11-12-13-14-15-16-17-21-37-26(35)19-18

InchiKey: BYRBTPGWKPEDMR-UHFFFAOYSA-N

Formula: C30H46F4O4

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

Mol. weight [g/mol]: 546.68

Physical Properties

Property code	Value	Unit	Source
gf	-971.47	kJ/mol	Joback Method
hf	-1745.92	kJ/mol	Joback Method
hfus	83.83	kJ/mol	Joback Method
hvap	102.34	kJ/mol	Joback Method
log10ws	-11.03		Crippen Method
logp	9.261		Crippen Method
mcvol	431.760	ml/mol	McGowan Method
pc	652.43	kPa	Joback Method
rinpol	3462.00		NIST Webbook
rinpol	3462.00		NIST Webbook
tb	1082.06	K	Joback Method
tc	1368.83	K	Joback Method
tf	651.04	K	Joback Method
vc	1.728	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1520.03	J/mol×K	1082.06	Joback Method
cpg	1539.53	J/mol×K	1129.86	Joback Method
cpg	1556.24	J/mol×K	1177.65	Joback Method
cpg	1570.25	J/mol×K	1225.45	Joback Method
cpg	1581.67	J/mol×K	1273.24	Joback Method
cpg	1590.62	J/mol×K	1321.04	Joback Method
cpg	1597.20	J/mol×K	1368.83	Joback Method

Sources

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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U377456&Units=SI

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