Glutaric acid, eicosyl 1-(pentafluorophenyl)ethyl ester

Inchi: InChI=1S/C33H51F5O4/c1-3-4-5-6-7-8-9-10-11-12-13-14-15-16-17-18-19-20-24-41-26(3

InchiKey: ABRVUIOYOOECMM-UHFFFAOYSA-N

Formula: C33H51F5O4

SMILES: CCCCCCCCCCCCCCCCCCCCCOC(=O)CCCC(=O)OC(C)c1c(F)c(F)c(F)c(F)c1F

Mol. weight [g/mol]: 606.75

Physical Properties

Property code	Value	Unit	Source
gf	-1153.09	kJ/mol	Joback Method
hf	-2020.70	kJ/mol	Joback Method
hfus	90.77	kJ/mol	Joback Method
hvap	108.48	kJ/mol	Joback Method
log10ws	-12.58		Crippen Method
logp	10.742		Crippen Method
mcvol	475.800	ml/mol	McGowan Method
pc	552.33	kPa	Joback Method
rinpol	3526.00		NIST Webbook
rinpol	3526.00		NIST Webbook
tb	1154.51	K	Joback Method
tc	1510.24	K	Joback Method
tf	682.96	K	Joback Method
vc	1.907	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1715.45	J/mol×K	1154.51	Joback Method
cpg	1736.16	J/mol×K	1213.80	Joback Method
cpg	1752.45	J/mol×K	1273.09	Joback Method
cpg	1764.54	J/mol×K	1332.37	Joback Method
cpg	1772.66	J/mol×K	1391.66	Joback Method
cpg	1777.05	J/mol×K	1450.95	Joback Method
cpg	1777.92	J/mol×K	1510.24	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U377013&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