Glutaric acid, octadecyl 1-(pentafluorophenyl)ethyl ester

Inchi: InChI=1S/C31H47F5O4/c1-3-4-5-6-7-8-9-10-11-12-13-14-15-16-17-18-22-39-24(37)20-1

InchiKey: XCBBIVURVMZQKH-UHFFFAOYSA-N

Formula: C31H47F5O4

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

Mol. weight [g/mol]: 578.69

Physical Properties

Property code	Value	Unit	Source
gf	-1169.93	kJ/mol	Joback Method
hf	-1979.42	kJ/mol	Joback Method
hfus	85.59	kJ/mol	Joback Method
hvap	104.02	kJ/mol	Joback Method
log10ws	-11.74		Crippen Method
logp	9.961		Crippen Method
mcvol	447.620	ml/mol	McGowan Method
pc	605.77	kPa	Joback Method
rinpol	3317.00		NIST Webbook
rinpol	3317.00		NIST Webbook
tb	1108.75	K	Joback Method
tc	1420.88	K	Joback Method
tf	660.42	K	Joback Method
vc	1.796	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1588.76	J/mol×K	1108.75	Joback Method
cpg	1608.49	J/mol×K	1160.77	Joback Method
cpg	1624.81	J/mol×K	1212.79	Joback Method
cpg	1637.83	J/mol×K	1264.82	Joback Method
cpg	1647.70	J/mol×K	1316.84	Joback Method
cpg	1654.55	J/mol×K	1368.86	Joback Method
cpg	1658.51	J/mol×K	1420.88	Joback Method

Sources

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=U377012&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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