Glutaric acid, heptadecyl 1-(pentafluorophenyl)ethyl ester

Inchi: InChI=1S/C30H45F5O4/c1-3-4-5-6-7-8-9-10-11-12-13-14-15-16-17-21-38-23(36)19-18-2

InchiKey: KSYZFNSAAONKLB-UHFFFAOYSA-N

Formula: C30H45F5O4

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

Mol. weight [g/mol]: 564.67

Physical Properties

Property code	Value	Unit	Source
gf	-1178.35	kJ/mol	Joback Method
hf	-1958.78	kJ/mol	Joback Method
hfus	83.00	kJ/mol	Joback Method
hvap	101.80	kJ/mol	Joback Method
log10ws	-11.33		Crippen Method
logp	9.571		Crippen Method
mcvol	433.530	ml/mol	McGowan Method
pc	635.44	kPa	Joback Method
rinpol	3212.00		NIST Webbook
tb	1085.87	K	Joback Method
tc	1379.43	K	Joback Method
tf	649.15	K	Joback Method
vc	1.740	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1525.62	J/mol×K	1085.87	Joback Method
cpg	1544.84	J/mol×K	1134.80	Joback Method
cpg	1561.05	J/mol×K	1183.72	Joback Method
cpg	1574.34	J/mol×K	1232.65	Joback Method
cpg	1584.81	J/mol×K	1281.58	Joback Method
cpg	1592.57	J/mol×K	1330.50	Joback Method
cpg	1597.73	J/mol×K	1379.43	Joback Method

Sources

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=U377011&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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