Glutaric acid, 2-(2-fluorophenyl)ethyl octadecyl ester

Inchi: InChI=1S/C31H51FO4/c1-2-3-4-5-6-7-8-9-10-11-12-13-14-15-16-19-26-35-30(33)23-20-2

InchiKey: HKNZYJHXQMKAIQ-UHFFFAOYSA-N

Formula: C31H51FO4

SMILES: CCCCCCCCCCCCCCCCCCOC(=O)CCCC(=O)OCCc1ccccc1F

Mol. weight [g/mol]: 506.73

Physical Properties

Property code	Value	Unit	Source
gf	-349.73	kJ/mol	Joback Method
hf	-1143.82	kJ/mol	Joback Method
hfus	78.35	kJ/mol	Joback Method
hvap	105.03	kJ/mol	Joback Method
log10ws	-9.96		Crippen Method
logp	8.886		Crippen Method
mcvol	440.540	ml/mol	McGowan Method
pc	681.36	kPa	Joback Method
rinpol	3631.00		NIST Webbook
rinpol	3631.00		NIST Webbook
tb	1092.19	K	Joback Method
tc	1365.18	K	Joback Method
tf	622.98	K	Joback Method
vc	1.730	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1567.20	J/mol×K	1092.19	Joback Method
cpg	1587.00	J/mol×K	1137.69	Joback Method
cpg	1604.41	J/mol×K	1183.19	Joback Method
cpg	1619.57	J/mol×K	1228.68	Joback Method
cpg	1632.60	J/mol×K	1274.18	Joback Method
cpg	1643.64	J/mol×K	1319.68	Joback Method
cpg	1652.82	J/mol×K	1365.18	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=U377098&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