Glutaric acid, oct-1-en-3-yl 2-fluorophenyl ester

Inchi: InChI=1S/C19H25FO4/c1-3-5-6-10-15(4-2)23-18(21)13-9-14-19(22)24-17-12-8-7-11-16(1

InchiKey: VYFZMZFEQCGVTC-UHFFFAOYSA-N

Formula: C19H25FO4

SMILES: C=CC(CCCCC)OC(=O)CCCC(=O)Oc1ccccc1F

Mol. weight [g/mol]: 336.40

Physical Properties

Property code	Value	Unit	Source
gf	-365.37	kJ/mol	Joback Method
hf	-775.99	kJ/mol	Joback Method
hfus	42.47	kJ/mol	Joback Method
hvap	77.26	kJ/mol	Joback Method
log10ws	-5.55		Crippen Method
logp	4.580		Crippen Method
mcvol	267.160	ml/mol	McGowan Method
pc	1446.83	kPa	Joback Method
rinpol	2224.00		NIST Webbook
rinpol	2224.00		NIST Webbook
tb	813.87	K	Joback Method
tc	1012.34	K	Joback Method
tf	470.98	K	Joback Method
vc	1.032	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	800.34	J/mol×K	813.87	Joback Method
cpg	815.44	J/mol×K	846.95	Joback Method
cpg	829.50	J/mol×K	880.03	Joback Method
cpg	842.55	J/mol×K	913.11	Joback Method
cpg	854.59	J/mol×K	946.19	Joback Method
cpg	865.67	J/mol×K	979.26	Joback Method
cpg	875.80	J/mol×K	1012.34	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=U405351&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