Glutaric acid, 2-fluorophenyl 2-methylhex-3-yl ester

Inchi: InChI=1S/C18H25FO4/c1-4-8-15(13(2)3)22-17(20)11-7-12-18(21)23-16-10-6-5-9-14(16)1

InchiKey: HVTSPRYJPONYOG-UHFFFAOYSA-N

Formula: C18H25FO4

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

Mol. weight [g/mol]: 324.39

Physical Properties

Property code	Value	Unit	Source
gf	-464.07	kJ/mol	Joback Method
hf	-886.06	kJ/mol	Joback Method
hfus	37.64	kJ/mol	Joback Method
hvap	75.32	kJ/mol	Joback Method
log10ws	-5.04		Crippen Method
logp	4.269		Crippen Method
mcvol	257.370	ml/mol	McGowan Method
pc	1517.57	kPa	Joback Method
rinpol	2087.00		NIST Webbook
rinpol	2087.00		NIST Webbook
tb	793.87	K	Joback Method
tc	992.71	K	Joback Method
tf	446.47	K	Joback Method
vc	0.990	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	769.87	J/mol×K	793.87	Joback Method
cpg	785.39	J/mol×K	827.01	Joback Method
cpg	799.85	J/mol×K	860.15	Joback Method
cpg	813.27	J/mol×K	893.29	Joback Method
cpg	825.66	J/mol×K	926.43	Joback Method
cpg	837.04	J/mol×K	959.57	Joback Method
cpg	847.43	J/mol×K	992.71	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=U393732&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