Glutaric acid, 1-(2,6-difluorophenyl)ethyl hexyl ester

Inchi: InChI=1S/C19H26F2O4/c1-3-4-5-6-13-24-17(22)11-8-12-18(23)25-14(2)19-15(20)9-7-10

InchiKey: ZOLYWIWIYLZGRT-UHFFFAOYSA-N

Formula: C19H26F2O4

SMILES: CCCCCCOC(=O)CCCC(=O)OC(C)c1c(F)cccc1F

Mol. weight [g/mol]: 356.40

Physical Properties

Property code	Value	Unit	Source
gf	-657.65	kJ/mol	Joback Method
hf	-1109.00	kJ/mol	Joback Method
hfus	46.44	kJ/mol	Joback Method
hvap	77.78	kJ/mol	Joback Method
log10ws	-5.73		Crippen Method
logp	4.863		Crippen Method
mcvol	273.230	ml/mol	McGowan Method
pc	1340.78	kPa	Joback Method
rinpol	2282.00		NIST Webbook
rinpol	2282.00		NIST Webbook
tb	821.44	K	Joback Method
tc	1015.17	K	Joback Method
tf	485.85	K	Joback Method
vc	1.069	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	833.81	J/mol×K	821.44	Joback Method
cpg	848.92	J/mol×K	853.73	Joback Method
cpg	863.00	J/mol×K	886.02	Joback Method
cpg	876.06	J/mol×K	918.30	Joback Method
cpg	888.12	J/mol×K	950.59	Joback Method
cpg	899.19	J/mol×K	982.88	Joback Method
cpg	909.29	J/mol×K	1015.17	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U377253&Units=SI
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

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