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

Inchi: InChI=1S/C18H24F2O4/c1-3-4-5-12-23-16(21)10-7-11-17(22)24-13(2)18-14(19)8-6-9-15

InchiKey: SHIYKUFDSNWINA-UHFFFAOYSA-N

Formula: C18H24F2O4

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

Mol. weight [g/mol]: 342.38

Physical Properties

Property code	Value	Unit	Source
gf	-666.07	kJ/mol	Joback Method
hf	-1088.36	kJ/mol	Joback Method
hfus	43.85	kJ/mol	Joback Method
hvap	75.55	kJ/mol	Joback Method
log10ws	-5.31		Crippen Method
logp	4.473		Crippen Method
mcvol	259.140	ml/mol	McGowan Method
pc	1440.25	kPa	Joback Method
rinpol	2181.00		NIST Webbook
rinpol	2181.00		NIST Webbook
tb	798.56	K	Joback Method
tc	991.38	K	Joback Method
tf	474.58	K	Joback Method
vc	1.014	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	776.15	J/mol×K	798.56	Joback Method
cpg	790.96	J/mol×K	830.70	Joback Method
cpg	804.79	J/mol×K	862.83	Joback Method
cpg	817.65	J/mol×K	894.97	Joback Method
cpg	829.56	J/mol×K	927.10	Joback Method
cpg	840.52	J/mol×K	959.24	Joback Method
cpg	850.54	J/mol×K	991.38	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=U377251&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