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

Inchi: InChI=1S/C26H40F2O4/c1-3-4-5-6-7-8-9-10-11-12-13-20-31-24(29)18-15-19-25(30)32-2

InchiKey: UWKOEWWNQVVUNJ-UHFFFAOYSA-N

Formula: C26H40F2O4

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

Mol. weight [g/mol]: 454.59

Physical Properties

Property code	Value	Unit	Source
gf	-598.71	kJ/mol	Joback Method
hf	-1253.48	kJ/mol	Joback Method
hfus	64.57	kJ/mol	Joback Method
hvap	93.36	kJ/mol	Joback Method
log10ws	-8.66		Crippen Method
logp	7.593		Crippen Method
mcvol	371.860	ml/mol	McGowan Method
pc	863.53	kPa	Joback Method
rinpol	2998.00		NIST Webbook
tb	981.60	K	Joback Method
tc	1204.73	K	Joback Method
tf	564.74	K	Joback Method
vc	1.462	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1257.04	J/mol×K	981.60	Joback Method
cpg	1274.34	J/mol×K	1018.79	Joback Method
cpg	1290.01	J/mol×K	1055.98	Joback Method
cpg	1304.12	J/mol×K	1093.16	Joback Method
cpg	1316.70	J/mol×K	1130.35	Joback Method
cpg	1327.81	J/mol×K	1167.54	Joback Method
cpg	1337.50	J/mol×K	1204.73	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U377258&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

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