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

Inchi: InChI=1S/C23H34F2O4/c1-3-4-5-6-7-8-9-10-17-28-21(26)15-12-16-22(27)29-18(2)23-19

InchiKey: GQWHSIBEFFMYRW-UHFFFAOYSA-N

Formula: C23H34F2O4

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

Mol. weight [g/mol]: 412.51

Physical Properties

Property code	Value	Unit	Source
gf	-623.97	kJ/mol	Joback Method
hf	-1191.56	kJ/mol	Joback Method
hfus	56.80	kJ/mol	Joback Method
hvap	86.68	kJ/mol	Joback Method
log10ws	-7.40		Crippen Method
logp	6.423		Crippen Method
mcvol	329.590	ml/mol	McGowan Method
pc	1030.59	kPa	Joback Method
rinpol	2686.00		NIST Webbook
rinpol	2686.00		NIST Webbook
tb	912.96	K	Joback Method
tc	1117.91	K	Joback Method
tf	530.93	K	Joback Method
vc	1.294	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1072.11	J/mol×K	912.96	Joback Method
cpg	1088.39	J/mol×K	947.12	Joback Method
cpg	1103.36	J/mol×K	981.28	Joback Method
cpg	1117.07	J/mol×K	1015.43	Joback Method
cpg	1129.54	J/mol×K	1049.59	Joback Method
cpg	1140.79	J/mol×K	1083.75	Joback Method
cpg	1150.86	J/mol×K	1117.91	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=U377255&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