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

Inchi: InChI=1S/C21H20F4O4/c1-12(20-14(22)6-3-7-15(20)23)28-18(26)10-5-11-19(27)29-13(2
InchiKey: CHIFOAZRJHRVLT-UHFFFAOYSA-N
Formula: C21H20F4O4
SMILES: CC(OC(=O)CCCC(=O)OC(C)c1c(F)cccc1F)c1c(F)cccc1F
Mol. weight [g/mol]: 412.37

Physical Properties

Property code	Value	Unit	Source
gf	-939.72	kJ/mol	Joback Method
hf	-1334.19	kJ/mol	Joback Method
hfus	47.52	kJ/mol	Joback Method
hvap	83.81	kJ/mol	Joback Method
log10ws	-6.79		Crippen Method
logp	5.322		Crippen Method
mcvol	281.190	ml/mol	McGowan Method
pc	1367.69	kPa	Joback Method
rinpol	2469.00		NIST Webbook
rinpol	2469.00		NIST Webbook
tb	901.94	K	Joback Method
tc	1112.05	K	Joback Method
tf	546.03	K	Joback Method
vc	1.103	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	865.81	J/mol×K	901.94	Joback Method
cpg	878.35	J/mol×K	936.96	Joback Method
cpg	889.70	J/mol×K	971.98	Joback Method
cpg	899.86	J/mol×K	1007.00	Joback Method
cpg	908.87	J/mol×K	1042.01	Joback Method
cpg	916.73	J/mol×K	1077.03	Joback Method
cpg	923.49	J/mol×K	1112.05	Joback Method

Sources

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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U377264&Units=SI

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