Glutaric acid, di(2-(4-fluorophenyl)ethyl) ester

Inchi: InChI=1S/C21H22F2O4/c22-18-8-4-16(5-9-18)12-14-26-20(24)2-1-3-21(25)27-15-13-17-
InchiKey: UPWSVNZEVYBERG-UHFFFAOYSA-N
Formula: C21H22F2O4
SMILES: O=C(CCCC(=O)OCCc1ccc(F)cc1)OCCc1ccc(F)cc1
Mol. weight [g/mol]: 376.39

Physical Properties

Property code	Value	Unit	Source
gf	-525.96	kJ/mol	Joback Method
hf	-908.47	kJ/mol	Joback Method
hfus	49.18	kJ/mol	Joback Method
hvap	84.89	kJ/mol	Joback Method
log10ws	-5.21		Crippen Method
logp	4.007		Crippen Method
mcvol	277.650	ml/mol	McGowan Method
pc	1479.29	kPa	Joback Method
rinpol	2718.00		NIST Webbook
rinpol	2718.00		NIST Webbook
tb	894.32	K	Joback Method
tc	1107.29	K	Joback Method
tf	549.81	K	Joback Method
vc	1.079	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	852.67	J/mol×K	894.32	Joback Method
cpg	865.98	J/mol×K	929.81	Joback Method
cpg	878.08	J/mol×K	965.31	Joback Method
cpg	889.02	J/mol×K	1000.80	Joback Method
cpg	898.83	J/mol×K	1036.30	Joback Method
cpg	907.54	J/mol×K	1071.79	Joback Method
cpg	915.18	J/mol×K	1107.29	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=U377129&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