Glutaric acid, 1-(cyclohex-2-enyl)hex-3-yl 2-fluorophenyl ester

Inchi: InChI=1S/C23H31FO4/c1-2-9-19(17-16-18-10-4-3-5-11-18)27-22(25)14-8-15-23(26)28-2

InchiKey: PLMXGJLCTDGFSQ-UHFFFAOYSA-N

Formula: C23H31FO4

SMILES: CCCC(CCC1C=CCCC1)OC(=O)CCCC(=O)Oc1ccccc1F

Mol. weight [g/mol]: 390.49

Physical Properties

Property code	Value	Unit	Source
gf	-365.12	kJ/mol	Joback Method
hf	-871.88	kJ/mol	Joback Method
hfus	47.17	kJ/mol	Joback Method
hvap	87.56	kJ/mol	Joback Method
log10ws	-6.88		Crippen Method
logp	5.750		Crippen Method
mcvol	312.660	ml/mol	McGowan Method
pc	1262.85	kPa	Joback Method
rinpol	2718.00		NIST Webbook
tb	927.42	K	Joback Method
tc	1144.16	K	Joback Method
tf	525.96	K	Joback Method
vc	1.194	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1030.59	J/mol×K	927.42	Joback Method
cpg	1046.37	J/mol×K	963.54	Joback Method
cpg	1060.65	J/mol×K	999.67	Joback Method
cpg	1073.48	J/mol×K	1035.79	Joback Method
cpg	1084.90	J/mol×K	1071.92	Joback Method
cpg	1094.95	J/mol×K	1108.04	Joback Method
cpg	1103.68	J/mol×K	1144.16	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U405516&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
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

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

Latest version available from:
https://www.chemeo.com/cid/99-132-6/Glutaric-acid-1-cyclohex-2-enyl-hex-3-yl-2-fluorophenyl-ester.pdf
Generated by Cheméo on 2024-04-29 00:39:29.543022619 +0000 UTC m=+16640418.463599941.
Cheméo (https://www.chemeo.com) is the biggest free database of chemical and physical data for the process industry.