Glutaric acid, 2-fluorophenyl 3-methyl-5-methoxypentyl ester

Inchi: InChI=1S/C18H25FO5/c1-14(10-12-22-2)11-13-23-17(20)8-5-9-18(21)24-16-7-4-3-6-15(1

InchiKey: SXPRFEOVWHWUAM-UHFFFAOYSA-N

Formula: C18H25FO5

SMILES: COCCC(C)CCOC(=O)CCCC(=O)Oc1ccccc1F

Mol. weight [g/mol]: 340.39

Physical Properties

Property code	Value	Unit	Source
gf	-566.63	kJ/mol	Joback Method
hf	-1013.00	kJ/mol	Joback Method
hfus	42.35	kJ/mol	Joback Method
hvap	78.12	kJ/mol	Joback Method
log10ws	-4.01		Crippen Method
logp	3.507		Crippen Method
mcvol	263.240	ml/mol	McGowan Method
pc	1488.44	kPa	Joback Method
rinpol	2306.00		NIST Webbook
rinpol	2306.00		NIST Webbook
tb	816.73	K	Joback Method
tc	1014.04	K	Joback Method
tf	483.70	K	Joback Method
vc	1.014	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	798.02	J/mol×K	816.73	Joback Method
cpg	812.96	J/mol×K	849.62	Joback Method
cpg	826.82	J/mol×K	882.50	Joback Method
cpg	839.60	J/mol×K	915.39	Joback Method
cpg	851.30	J/mol×K	948.27	Joback Method
cpg	861.93	J/mol×K	981.16	Joback Method
cpg	871.50	J/mol×K	1014.04	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U393524&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/99-543-0/Glutaric-acid-2-fluorophenyl-3-methyl-5-methoxypentyl-ester.pdf
Generated by Cheméo on 2024-04-28 22:34:11.449859956 +0000 UTC m=+16632900.370437268.
Cheméo (https://www.chemeo.com) is the biggest free database of chemical and physical data for the process industry.