Glutaric acid, 2-fluorophenyl 4-cyanophenyl ester

Inchi: InChI=1S/C18H14FNO4/c19-15-4-1-2-5-16(15)24-18(22)7-3-6-17(21)23-14-10-8-13(12-2

InchiKey: KVYAJCPBAMCFGI-UHFFFAOYSA-N

Formula: C18H14FNO4

SMILES: N#Cc1ccc(OC(=O)CCCC(=O)Oc2ccccc2F)cc1

Mol. weight [g/mol]: 327.31

Physical Properties

Property code	Value	Unit	Source
gf	-223.23	kJ/mol	Joback Method
hf	-485.56	kJ/mol	Joback Method
hfus	39.84	kJ/mol	Joback Method
hvap	89.51	kJ/mol	Joback Method
log10ws	-4.85		Crippen Method
logp	3.379		Crippen Method
mcvol	234.990	ml/mol	McGowan Method
pc	1903.58	kPa	Joback Method
rinpol	2674.00		NIST Webbook
rinpol	2674.00		NIST Webbook
tb	928.49	K	Joback Method
tc	1161.78	K	Joback Method
tf	580.40	K	Joback Method
vc	0.919	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	686.48	J/mol×K	928.49	Joback Method
cpg	696.19	J/mol×K	967.37	Joback Method
cpg	704.72	J/mol×K	1006.25	Joback Method
cpg	712.09	J/mol×K	1045.13	Joback Method
cpg	718.35	J/mol×K	1084.02	Joback Method
cpg	723.50	J/mol×K	1122.90	Joback Method
cpg	727.59	J/mol×K	1161.78	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=U393275&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

Latest version available from:
https://www.chemeo.com/cid/73-791-3/Glutaric-acid-2-fluorophenyl-4-cyanophenyl-ester.pdf
Generated by Cheméo on 2024-04-19 15:36:46.440517855 +0000 UTC m=+15830255.361095170.
Cheméo (https://www.chemeo.com) is the biggest free database of chemical and physical data for the process industry.