Glutaric acid, hex-2-en-1-yl 2-fluorophenyl ester

Inchi: InChI=1S/C17H21FO4/c1-2-3-4-7-13-21-16(19)11-8-12-17(20)22-15-10-6-5-9-14(15)18/h

InchiKey: ZUGMGQXQEJTUBV-QPJJXVBHSA-N

Formula: C17H21FO4

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

Mol. weight [g/mol]: 308.34

Physical Properties

Property code	Value	Unit	Source
gf	-387.39	kJ/mol	Joback Method
hf	-737.64	kJ/mol	Joback Method
hfus	42.29	kJ/mol	Joback Method
hvap	73.83	kJ/mol	Joback Method
log10ws	-4.60		Crippen Method
logp	3.801		Crippen Method
mcvol	238.980	ml/mol	McGowan Method
pc	1686.56	kPa	Joback Method
rinpol	2132.00		NIST Webbook
rinpol	2132.00		NIST Webbook
tb	776.03	K	Joback Method
tc	975.93	K	Joback Method
tf	460.12	K	Joback Method
vc	0.925	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	686.98	J/mol×K	776.03	Joback Method
cpg	701.35	J/mol×K	809.35	Joback Method
cpg	714.78	J/mol×K	842.66	Joback Method
cpg	727.30	J/mol×K	875.98	Joback Method
cpg	738.93	J/mol×K	909.30	Joback Method
cpg	749.71	J/mol×K	942.62	Joback Method
cpg	759.66	J/mol×K	975.93	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=U405331&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