Glutaric acid, but-3-en-2-yl 2-fluorophenyl ester

Inchi: InChI=1S/C15H17FO4/c1-3-11(2)19-14(17)9-6-10-15(18)20-13-8-5-4-7-12(13)16/h3-5,7-

InchiKey: KTPSTWNRORUSPW-UHFFFAOYSA-N

Formula: C15H17FO4

SMILES: C=CC(C)OC(=O)CCCC(=O)Oc1ccccc1F

Mol. weight [g/mol]: 280.29

Physical Properties

Property code	Value	Unit	Source
gf	-399.05	kJ/mol	Joback Method
hf	-693.43	kJ/mol	Joback Method
hfus	32.11	kJ/mol	Joback Method
hvap	68.36	kJ/mol	Joback Method
log10ws	-3.88		Crippen Method
logp	3.019		Crippen Method
mcvol	210.800	ml/mol	McGowan Method
pc	1984.12	kPa	Joback Method
rinpol	1848.00		NIST Webbook
rinpol	1848.00		NIST Webbook
tb	722.35	K	Joback Method
tc	924.80	K	Joback Method
tf	425.90	K	Joback Method
vc	0.808	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	577.66	J/mol×K	722.35	Joback Method
cpg	591.52	J/mol×K	756.09	Joback Method
cpg	604.49	J/mol×K	789.83	Joback Method
cpg	616.56	J/mol×K	823.58	Joback Method
cpg	627.76	J/mol×K	857.32	Joback Method
cpg	638.10	J/mol×K	891.06	Joback Method
cpg	647.59	J/mol×K	924.80	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U405238&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

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