Glutaric acid, 3-methylbut-2-yl 3-fluorophenyl ester

Inchi: InChI=1S/C16H21FO4/c1-11(2)12(3)20-15(18)8-5-9-16(19)21-14-7-4-6-13(17)10-14/h4,6

InchiKey: LLQCVIDSEBTKIO-UHFFFAOYSA-N

Formula: C16H21FO4

SMILES: CC(C)C(C)OC(=O)CCCC(=O)Oc1cccc(F)c1

Mol. weight [g/mol]: 296.33

Physical Properties

Property code	Value	Unit	Source
gf	-480.91	kJ/mol	Joback Method
hf	-844.78	kJ/mol	Joback Method
hfus	32.46	kJ/mol	Joback Method
hvap	70.87	kJ/mol	Joback Method
log10ws	-4.20		Crippen Method
logp	3.489		Crippen Method
mcvol	229.190	ml/mol	McGowan Method
pc	1772.85	kPa	Joback Method
rinpol	1924.00		NIST Webbook
rinpol	1924.00		NIST Webbook
tb	748.11	K	Joback Method
tc	948.92	K	Joback Method
tf	423.93	K	Joback Method
vc	0.877	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	657.27	J/mol×K	748.11	Joback Method
cpg	672.26	J/mol×K	781.58	Joback Method
cpg	686.26	J/mol×K	815.05	Joback Method
cpg	699.29	J/mol×K	848.52	Joback Method
cpg	711.36	J/mol×K	881.98	Joback Method
cpg	722.47	J/mol×K	915.45	Joback Method
cpg	732.65	J/mol×K	948.92	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=U392087&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