Glutaric acid, butyl 1-(4-fluorophenyl)ethyl ester

Inchi: InChI=1S/C17H23FO4/c1-3-4-12-21-16(19)6-5-7-17(20)22-13(2)14-8-10-15(18)11-9-14/h

InchiKey: ODPJDRXLHULCLD-UHFFFAOYSA-N

Formula: C17H23FO4

SMILES: CCCCOC(=O)CCCC(=O)OC(C)c1ccc(F)cc1

Mol. weight [g/mol]: 310.36

Physical Properties

Property code	Value	Unit	Source
gf	-470.05	kJ/mol	Joback Method
hf	-860.14	kJ/mol	Joback Method
hfus	38.57	kJ/mol	Joback Method
hvap	73.48	kJ/mol	Joback Method
log10ws	-4.56		Crippen Method
logp	3.943		Crippen Method
mcvol	243.280	ml/mol	McGowan Method
pc	1627.22	kPa	Joback Method
rinpol	2084.00		NIST Webbook
tb	771.43	K	Joback Method
tc	968.49	K	Joback Method
tf	450.20	K	Joback Method
vc	0.940	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	712.53	J/mol×K	771.43	Joback Method
cpg	727.61	J/mol×K	804.27	Joback Method
cpg	741.70	J/mol×K	837.12	Joback Method
cpg	754.82	J/mol×K	869.96	Joback Method
cpg	766.97	J/mol×K	902.80	Joback Method
cpg	778.18	J/mol×K	935.65	Joback Method
cpg	788.46	J/mol×K	968.49	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U377102&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

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