Glutaric acid, 3-methylbut-2-yl 4-fluoro-2-methoxyphenyl ester

Inchi: InChI=1S/C17H23FO5/c1-11(2)12(3)22-16(19)6-5-7-17(20)23-14-9-8-13(18)10-15(14)21
InchiKey: OENMUHAQEFBWMM-UHFFFAOYSA-N
Formula: C17H23FO5
SMILES: COc1cc(F)ccc1OC(=O)CCCC(=O)OC(C)C(C)C
Mol. weight [g/mol]: 326.36

Physical Properties

Property code	Value	Unit	Source
gf	-587.12	kJ/mol	Joback Method
hf	-1009.11	kJ/mol	Joback Method
hfus	35.84	kJ/mol	Joback Method
hvap	76.17	kJ/mol	Joback Method
log10ws	-4.32		Crippen Method
logp	3.498		Crippen Method
mcvol	249.150	ml/mol	McGowan Method
pc	1596.17	kPa	Joback Method
rinpol	2111.00		NIST Webbook
rinpol	2111.00		NIST Webbook
tb	798.39	K	Joback Method
tc	998.63	K	Joback Method
tf	469.95	K	Joback Method
vc	0.952	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	740.51	J/mol×K	798.39	Joback Method
cpg	755.28	J/mol×K	831.76	Joback Method
cpg	768.98	J/mol×K	865.14	Joback Method
cpg	781.62	J/mol×K	898.51	Joback Method
cpg	793.18	J/mol×K	931.88	Joback Method
cpg	803.67	J/mol×K	965.25	Joback Method
cpg	813.09	J/mol×K	998.63	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U393440&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
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

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