Glutaric acid, ethyl 3-fluorophenyl ester

Inchi: InChI=1S/C13H15FO4/c1-2-17-12(15)7-4-8-13(16)18-11-6-3-5-10(14)9-11/h3,5-6,9H,2,4
InchiKey: LHXKZPNXQXNEMH-UHFFFAOYSA-N
Formula: C13H15FO4
SMILES: CCOC(=O)CCCC(=O)Oc1cccc(F)c1
Mol. weight [g/mol]: 254.25

Physical Properties

Property code	Value	Unit	Source
gf	-501.29	kJ/mol	Joback Method
hf	-772.30	kJ/mol	Joback Method
hfus	31.73	kJ/mol	Joback Method
hvap	64.97	kJ/mol	Joback Method
log10ws	-3.07		Crippen Method
logp	2.464		Crippen Method
mcvol	186.920	ml/mol	McGowan Method
pc	2261.11	kPa	Joback Method
rinpol	1782.00		NIST Webbook
rinpol	1782.00		NIST Webbook
tb	680.35	K	Joback Method
tc	880.81	K	Joback Method
tf	420.12	K	Joback Method
vc	0.722	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	495.55	J/mol×K	680.35	Joback Method
cpg	508.85	J/mol×K	713.76	Joback Method
cpg	521.34	J/mol×K	747.17	Joback Method
cpg	533.05	J/mol×K	780.58	Joback Method
cpg	543.96	J/mol×K	813.99	Joback Method
cpg	554.09	J/mol×K	847.40	Joback Method
cpg	563.45	J/mol×K	880.81	Joback Method

Sources

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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U359045&Units=SI

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