Glutaric acid, 2-fluorophenyl phenethyl ester

Inchi: InChI=1S/C19H19FO4/c20-16-9-4-5-10-17(16)24-19(22)12-6-11-18(21)23-14-13-15-7-2-
InchiKey: ACYRBLYKPHFCJK-UHFFFAOYSA-N
Formula: C19H19FO4
SMILES: O=C(CCCC(=O)Oc1ccccc1F)OCCc1ccccc1
Mol. weight [g/mol]: 330.35

Physical Properties

Property code	Value	Unit	Source
gf	-338.36	kJ/mol	Joback Method
hf	-659.61	kJ/mol	Joback Method
hfus	41.31	kJ/mol	Joback Method
hvap	80.60	kJ/mol	Joback Method
log10ws	-4.69		Crippen Method
logp	3.687		Crippen Method
mcvol	247.700	ml/mol	McGowan Method
pc	1813.86	kPa	Joback Method
rinpol	2459.00		NIST Webbook
rinpol	2459.00		NIST Webbook
tb	844.31	K	Joback Method
tc	1063.19	K	Joback Method
tf	514.16	K	Joback Method
vc	0.950	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	731.86	J/mol×K	844.31	Joback Method
cpg	745.41	J/mol×K	880.79	Joback Method
cpg	757.77	J/mol×K	917.27	Joback Method
cpg	768.98	J/mol×K	953.75	Joback Method
cpg	779.06	J/mol×K	990.23	Joback Method
cpg	788.06	J/mol×K	1026.71	Joback Method
cpg	796.00	J/mol×K	1063.19	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=U391791&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