Glutaric acid, naphth-2-ylmethyl 3-fluorophenyl ester

Inchi: InChI=1S/C22H19FO4/c23-19-7-3-8-20(14-19)27-22(25)10-4-9-21(24)26-15-16-11-12-17

InchiKey: LYXSNYGHZGLCPB-UHFFFAOYSA-N

Formula: C22H19FO4

SMILES: O=C(CCCC(=O)Oc1cccc(F)c1)OCc1ccc2ccccc2c1

Mol. weight [g/mol]: 366.38

Physical Properties

Property code	Value	Unit	Source
gf	-216.08	kJ/mol	Joback Method
hf	-541.93	kJ/mol	Joback Method
hfus	45.71	kJ/mol	Joback Method
hvap	89.58	kJ/mol	Joback Method
log10ws	-6.57		Crippen Method
logp	4.798		Crippen Method
mcvol	270.510	ml/mol	McGowan Method
pc	1727.46	kPa	Joback Method
rinpol	3054.00		NIST Webbook
rinpol	3054.00		NIST Webbook
tb	936.91	K	Joback Method
tc	1169.23	K	Joback Method
tf	593.19	K	Joback Method
vc	1.040	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	823.04	J/mol×K	936.91	Joback Method
cpg	835.36	J/mol×K	975.63	Joback Method
cpg	846.54	J/mol×K	1014.35	Joback Method
cpg	856.66	J/mol×K	1053.07	Joback Method
cpg	865.80	J/mol×K	1091.79	Joback Method
cpg	874.02	J/mol×K	1130.51	Joback Method
cpg	881.41	J/mol×K	1169.23	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=U392101&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