Glutaric acid, naphth-2-ylmethyl 4-fluoro-2-methoxyphenyl ester

Inchi: InChI=1S/C23H21FO5/c1-27-21-14-19(24)11-12-20(21)29-23(26)8-4-7-22(25)28-15-16-9

InchiKey: FUAMMMQROHURBX-UHFFFAOYSA-N

Formula: C23H21FO5

SMILES: COc1cc(F)ccc1OC(=O)CCCC(=O)OCc1ccc2ccccc2c1

Mol. weight [g/mol]: 396.41

Physical Properties

Property code	Value	Unit	Source
gf	-322.29	kJ/mol	Joback Method
hf	-706.26	kJ/mol	Joback Method
hfus	49.10	kJ/mol	Joback Method
hvap	94.88	kJ/mol	Joback Method
log10ws	-6.69		Crippen Method
logp	4.807		Crippen Method
mcvol	290.470	ml/mol	McGowan Method
pc	1557.35	kPa	Joback Method
rinpol	3210.00		NIST Webbook
rinpol	3210.00		NIST Webbook
tb	987.19	K	Joback Method
tc	1220.03	K	Joback Method
tf	639.21	K	Joback Method
vc	1.113	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	905.64	J/mol×K	987.19	Joback Method
cpg	917.11	J/mol×K	1026.00	Joback Method
cpg	927.28	J/mol×K	1064.80	Joback Method
cpg	936.20	J/mol×K	1103.61	Joback Method
cpg	943.92	J/mol×K	1142.42	Joback Method
cpg	950.50	J/mol×K	1181.23	Joback Method
cpg	955.97	J/mol×K	1220.03	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=U393570&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