Glutaric acid, naphth-2-ylmethyl 2,3,4-trifluorophenyl ester

Inchi: InChI=1S/C22H17F3O4/c23-17-10-11-18(22(25)21(17)24)29-20(27)7-3-6-19(26)28-13-14

InchiKey: SYLLXGPNGWWROY-UHFFFAOYSA-N

Formula: C22H17F3O4

SMILES: O=C(CCCC(=O)Oc1ccc(F)c(F)c1F)OCc1ccc2ccccc2c1

Mol. weight [g/mol]: 402.36

Physical Properties

Property code	Value	Unit	Source
gf	-624.96	kJ/mol	Joback Method
hf	-957.09	kJ/mol	Joback Method
hfus	51.09	kJ/mol	Joback Method
hvap	89.27	kJ/mol	Joback Method
log10ws	-7.23		Crippen Method
logp	5.076		Crippen Method
mcvol	274.050	ml/mol	McGowan Method
pc	1567.23	kPa	Joback Method
rinpol	2954.00		NIST Webbook
tb	945.41	K	Joback Method
tc	1169.07	K	Joback Method
tf	619.41	K	Joback Method
vc	1.075	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	834.34	J/mol×K	945.41	Joback Method
cpg	845.68	J/mol×K	982.69	Joback Method
cpg	855.95	J/mol×K	1019.96	Joback Method
cpg	865.20	J/mol×K	1057.24	Joback Method
cpg	873.49	J/mol×K	1094.51	Joback Method
cpg	880.86	J/mol×K	1131.79	Joback Method
cpg	887.37	J/mol×K	1169.07	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U393650&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