Glutaric acid, naphth-2-ylmethyl pentafluorophenyl ester

Inchi: InChI=1S/C22H15F5O4/c23-17-18(24)20(26)22(21(27)19(17)25)31-16(29)7-3-6-15(28)3
InchiKey: RXUPBGCPWSRBMO-UHFFFAOYSA-N
Formula: C22H15F5O4
SMILES: O=C(CCCC(=O)Oc1c(F)c(F)c(F)c(F)c1F)OCc1ccc2ccccc2c1
Mol. weight [g/mol]: 438.34

Physical Properties

Property code	Value	Unit	Source
gf	-1033.84	kJ/mol	Joback Method
hf	-1372.25	kJ/mol	Joback Method
hfus	56.48	kJ/mol	Joback Method
hvap	88.96	kJ/mol	Joback Method
log10ws	-7.89		Crippen Method
logp	5.354		Crippen Method
mcvol	277.590	ml/mol	McGowan Method
pc	1428.30	kPa	Joback Method
rinpol	2782.00		NIST Webbook
rinpol	2782.00		NIST Webbook
tb	953.91	K	Joback Method
tc	1172.31	K	Joback Method
tf	645.63	K	Joback Method
vc	1.111	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	845.46	J/mol×K	953.91	Joback Method
cpg	856.01	J/mol×K	990.31	Joback Method
cpg	865.52	J/mol×K	1026.71	Joback Method
cpg	874.02	J/mol×K	1063.11	Joback Method
cpg	881.55	J/mol×K	1099.51	Joback Method
cpg	888.14	J/mol×K	1135.91	Joback Method
cpg	893.84	J/mol×K	1172.31	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U392118&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

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