Glutaric acid, dec-2-yl 4-cyanophenyl ester

Inchi: InChI=1S/C22H31NO4/c1-3-4-5-6-7-8-10-18(2)26-21(24)11-9-12-22(25)27-20-15-13-19(
InchiKey: BPJYEEYNIRWFPC-UHFFFAOYSA-N
Formula: C22H31NO4
SMILES: CCCCCCCCC(C)OC(=O)CCCC(=O)Oc1ccc(C#N)cc1
Mol. weight [g/mol]: 373.49

Physical Properties

Property code	Value	Unit	Source
gf	-99.96	kJ/mol	Joback Method
hf	-602.35	kJ/mol	Joback Method
hfus	49.95	kJ/mol	Joback Method
hvap	95.91	kJ/mol	Joback Method
log10ws	-6.55		Crippen Method
logp	5.316		Crippen Method
mcvol	313.340	ml/mol	McGowan Method
pc	1157.71	kPa	Joback Method
rinpol	2819.00		NIST Webbook
rinpol	2819.00		NIST Webbook
tb	988.64	K	Joback Method
tc	1211.56	K	Joback Method
tf	570.95	K	Joback Method
vc	1.228	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1020.62	J/mol×K	988.64	Joback Method
cpg	1033.88	J/mol×K	1025.79	Joback Method
cpg	1045.78	J/mol×K	1062.95	Joback Method
cpg	1056.36	J/mol×K	1100.10	Joback Method
cpg	1065.66	J/mol×K	1137.25	Joback Method
cpg	1073.72	J/mol×K	1174.41	Joback Method
cpg	1080.56	J/mol×K	1211.56	Joback Method

Sources

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=U393279&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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