Glutaric acid, di(4-cyanophenyl) ester

Inchi: InChI=1S/C19H14N2O4/c20-12-14-4-8-16(9-5-14)24-18(22)2-1-3-19(23)25-17-10-6-15(1
InchiKey: GQADUDRHRQFMRI-UHFFFAOYSA-N
Formula: C19H14N2O4
SMILES: N#Cc1ccc(OC(=O)CCCC(=O)Oc2ccc(C#N)cc2)cc1
Mol. weight [g/mol]: 334.33

Physical Properties

Property code	Value	Unit	Source
gf	113.18	kJ/mol	Joback Method
hf	-145.21	kJ/mol	Joback Method
hfus	40.86	kJ/mol	Joback Method
hvap	103.03	kJ/mol	Joback Method
log10ws	-4.87		Crippen Method
logp	3.111		Crippen Method
mcvol	248.690	ml/mol	McGowan Method
pc	1783.35	kPa	Joback Method
rinpol	3190.00		NIST Webbook
tb	1054.18	K	Joback Method
tc	1304.79	K	Joback Method
tf	656.07	K	Joback Method
vc	0.984	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	734.84	J/mol×K	1054.18	Joback Method
cpg	741.36	J/mol×K	1095.95	Joback Method
cpg	746.60	J/mol×K	1137.72	Joback Method
cpg	750.59	J/mol×K	1179.48	Joback Method
cpg	753.36	J/mol×K	1221.25	Joback Method
cpg	754.95	J/mol×K	1263.02	Joback Method
cpg	755.40	J/mol×K	1304.79	Joback Method

Sources

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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U358624&Units=SI

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