Glutaric acid, 4-cyanophenyl ethyl ester

Inchi: InChI=1S/C14H15NO4/c1-2-18-13(16)4-3-5-14(17)19-12-8-6-11(10-15)7-9-12/h6-9H,2-5
InchiKey: RJYLVFHPOHIKBX-UHFFFAOYSA-N
Formula: C14H15NO4
SMILES: CCOC(=O)CCCC(=O)Oc1ccc(C#N)cc1
Mol. weight [g/mol]: 261.27

Physical Properties

Property code	Value	Unit	Source
gf	-164.88	kJ/mol	Joback Method
hf	-431.95	kJ/mol	Joback Method
hfus	32.75	kJ/mol	Joback Method
hvap	78.49	kJ/mol	Joback Method
log10ws	-3.09		Crippen Method
logp	2.197		Crippen Method
mcvol	200.620	ml/mol	McGowan Method
pc	2106.13	kPa	Joback Method
rinpol	2137.00		NIST Webbook
rinpol	2137.00		NIST Webbook
tb	806.04	K	Joback Method
tc	1023.99	K	Joback Method
tf	495.79	K	Joback Method
vc	0.785	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	561.40	J/mol×K	806.04	Joback Method
cpg	572.81	J/mol×K	842.37	Joback Method
cpg	583.29	J/mol×K	878.69	Joback Method
cpg	592.83	J/mol×K	915.02	Joback Method
cpg	601.45	J/mol×K	951.34	Joback Method
cpg	609.15	J/mol×K	987.67	Joback Method
cpg	615.93	J/mol×K	1023.99	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U358609&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