Glutaric acid, butyl 4-cyanophenyl ester

Inchi: InChI=1S/C16H19NO4/c1-2-3-11-20-15(18)5-4-6-16(19)21-14-9-7-13(12-17)8-10-14/h7-1
InchiKey: YARCBKWABQXNIG-UHFFFAOYSA-N
Formula: C16H19NO4
SMILES: CCCCOC(=O)CCCC(=O)Oc1ccc(C#N)cc1
Mol. weight [g/mol]: 289.33

Physical Properties

Property code	Value	Unit	Source
gf	-148.04	kJ/mol	Joback Method
hf	-473.23	kJ/mol	Joback Method
hfus	37.93	kJ/mol	Joback Method
hvap	82.94	kJ/mol	Joback Method
log10ws	-3.93		Crippen Method
logp	2.977		Crippen Method
mcvol	228.800	ml/mol	McGowan Method
pc	1778.84	kPa	Joback Method
rinpol	2347.00		NIST Webbook
tb	851.80	K	Joback Method
tc	1066.43	K	Joback Method
tf	518.33	K	Joback Method
vc	0.897	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	671.42	J/mol×K	851.80	Joback Method
cpg	683.46	J/mol×K	887.57	Joback Method
cpg	694.48	J/mol×K	923.34	Joback Method
cpg	704.50	J/mol×K	959.11	Joback Method
cpg	713.53	J/mol×K	994.88	Joback Method
cpg	721.57	J/mol×K	1030.65	Joback Method
cpg	728.64	J/mol×K	1066.43	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=U358612&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