Glutaric acid, 4-cyanophenyl isohexyl ester

Inchi: InChI=1S/C18H23NO4/c1-14(2)5-4-12-22-17(20)6-3-7-18(21)23-16-10-8-15(13-19)9-11-
InchiKey: RESKHSMHNKVIHS-UHFFFAOYSA-N
Formula: C18H23NO4
SMILES: CC(C)CCCOC(=O)CCCC(=O)Oc1ccc(C#N)cc1
Mol. weight [g/mol]: 317.38

Physical Properties

Property code	Value	Unit	Source
gf	-133.64	kJ/mol	Joback Method
hf	-519.79	kJ/mol	Joback Method
hfus	39.59	kJ/mol	Joback Method
hvap	87.00	kJ/mol	Joback Method
log10ws	-4.53		Crippen Method
logp	3.613		Crippen Method
mcvol	256.980	ml/mol	McGowan Method
pc	1531.86	kPa	Joback Method
rinpol	2518.00		NIST Webbook
rinpol	2518.00		NIST Webbook
tb	897.12	K	Joback Method
tc	1113.04	K	Joback Method
tf	525.87	K	Joback Method
vc	1.004	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	785.45	J/mol×K	897.12	Joback Method
cpg	798.05	J/mol×K	933.11	Joback Method
cpg	809.51	J/mol×K	969.09	Joback Method
cpg	819.85	J/mol×K	1005.08	Joback Method
cpg	829.09	J/mol×K	1041.06	Joback Method
cpg	837.26	J/mol×K	1077.05	Joback Method
cpg	844.37	J/mol×K	1113.04	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U358614&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