Glutaric acid, 4-cyanophenyl pentadecyl ester

Inchi: InChI=1S/C27H41NO4/c1-2-3-4-5-6-7-8-9-10-11-12-13-14-22-31-26(29)16-15-17-27(30)
InchiKey: QMDVVXJDKFBDKQ-UHFFFAOYSA-N
Formula: C27H41NO4
SMILES: CCCCCCCCCCCCCCCOC(=O)CCCC(=O)Oc1ccc(C#N)cc1
Mol. weight [g/mol]: 443.62

Physical Properties

Property code	Value	Unit	Source
gf	-55.42	kJ/mol	Joback Method
hf	-700.27	kJ/mol	Joback Method
hfus	66.42	kJ/mol	Joback Method
hvap	107.42	kJ/mol	Joback Method
log10ws	-8.54		Crippen Method
logp	7.268		Crippen Method
mcvol	383.790	ml/mol	McGowan Method
pc	851.47	kPa	Joback Method
rinpol	3529.00		NIST Webbook
tb	1103.48	K	Joback Method
tc	1359.96	K	Joback Method
tf	642.30	K	Joback Method
vc	1.514	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1325.33	J/mol×K	1103.48	Joback Method
cpg	1339.73	J/mol×K	1146.23	Joback Method
cpg	1352.26	J/mol×K	1188.97	Joback Method
cpg	1363.01	J/mol×K	1231.72	Joback Method
cpg	1372.05	J/mol×K	1274.47	Joback Method
cpg	1379.47	J/mol×K	1317.22	Joback Method
cpg	1385.36	J/mol×K	1359.96	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=U358623&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

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