Glutaric acid, 4-cyanophenyl pentyl ester

Inchi: InChI=1S/C17H21NO4/c1-2-3-4-12-21-16(19)6-5-7-17(20)22-15-10-8-14(13-18)9-11-15/h
InchiKey: VEAFCYKFLPSZJY-UHFFFAOYSA-N
Formula: C17H21NO4
SMILES: CCCCCOC(=O)CCCC(=O)Oc1ccc(C#N)cc1
Mol. weight [g/mol]: 303.35

Physical Properties

Property code	Value	Unit	Source
gf	-139.62	kJ/mol	Joback Method
hf	-493.87	kJ/mol	Joback Method
hfus	40.52	kJ/mol	Joback Method
hvap	85.16	kJ/mol	Joback Method
log10ws	-4.35		Crippen Method
logp	3.367		Crippen Method
mcvol	242.890	ml/mol	McGowan Method
pc	1643.09	kPa	Joback Method
rinpol	2454.00		NIST Webbook
tb	874.68	K	Joback Method
tc	1088.63	K	Joback Method
tf	529.60	K	Joback Method
vc	0.954	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	727.77	J/mol×K	874.68	Joback Method
cpg	740.06	J/mol×K	910.34	Joback Method
cpg	751.30	J/mol×K	946.00	Joback Method
cpg	761.49	J/mol×K	981.66	Joback Method
cpg	770.65	J/mol×K	1017.32	Joback Method
cpg	778.79	J/mol×K	1052.97	Joback Method
cpg	785.94	J/mol×K	1088.63	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=U358613&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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