Glutaric acid, 2-ethylhexyl 4-cyanophenyl ester

Inchi: InChI=1S/C20H27NO4/c1-3-5-7-16(4-2)15-24-19(22)8-6-9-20(23)25-18-12-10-17(14-21)
InchiKey: PNUDLLIBKNIMPR-UHFFFAOYSA-N
Formula: C20H27NO4
SMILES: CCCCC(CC)COC(=O)CCCC(=O)Oc1ccc(C#N)cc1
Mol. weight [g/mol]: 345.43

Physical Properties

Property code	Value	Unit	Source
gf	-116.80	kJ/mol	Joback Method
hf	-561.07	kJ/mol	Joback Method
hfus	44.76	kJ/mol	Joback Method
hvap	91.45	kJ/mol	Joback Method
log10ws	-5.36		Crippen Method
logp	4.394		Crippen Method
mcvol	285.160	ml/mol	McGowan Method
pc	1325.20	kPa	Joback Method
rinpol	2754.00		NIST Webbook
rinpol	2754.00		NIST Webbook
tb	942.88	K	Joback Method
tc	1160.56	K	Joback Method
tf	548.41	K	Joback Method
vc	1.115	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	901.82	J/mol×K	942.88	Joback Method
cpg	914.76	J/mol×K	979.16	Joback Method
cpg	926.47	J/mol×K	1015.44	Joback Method
cpg	936.97	J/mol×K	1051.72	Joback Method
cpg	946.30	J/mol×K	1088.00	Joback Method
cpg	954.47	J/mol×K	1124.28	Joback Method
cpg	961.51	J/mol×K	1160.56	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U393276&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

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