Glutaric acid, cyclohexylmethyl 4-cyanophenyl ester

Inchi: InChI=1S/C19H23NO4/c20-13-15-9-11-17(12-10-15)24-19(22)8-4-7-18(21)23-14-16-5-2-
InchiKey: NCIIMKSUQCAWIJ-UHFFFAOYSA-N
Formula: C19H23NO4
SMILES: N#Cc1ccc(OC(=O)CCCC(=O)OCC2CCCCC2)cc1
Mol. weight [g/mol]: 329.39

Physical Properties

Property code	Value	Unit	Source
gf	-98.33	kJ/mol	Joback Method
hf	-480.83	kJ/mol	Joback Method
hfus	37.53	kJ/mol	Joback Method
hvap	90.04	kJ/mol	Joback Method
log10ws	-4.84		Crippen Method
logp	3.757		Crippen Method
mcvol	260.210	ml/mol	McGowan Method
pc	1660.55	kPa	Joback Method
rinpol	2053.00		NIST Webbook
rinpol	2053.00		NIST Webbook
tb	939.99	K	Joback Method
tc	1172.93	K	Joback Method
tf	559.52	K	Joback Method
vc	0.999	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	835.44	J/mol×K	939.99	Joback Method
cpg	848.24	J/mol×K	978.81	Joback Method
cpg	859.53	J/mol×K	1017.64	Joback Method
cpg	869.36	J/mol×K	1056.46	Joback Method
cpg	877.75	J/mol×K	1095.28	Joback Method
cpg	884.74	J/mol×K	1134.10	Joback Method
cpg	890.37	J/mol×K	1172.93	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U393234&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