Glutaric acid, 2-methylpent-3-yl 4-cyanophenyl ester

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

Physical Properties

Property code	Value	Unit	Source
gf	-136.08	kJ/mol	Joback Method
hf	-525.07	kJ/mol	Joback Method
hfus	36.06	kJ/mol	Joback Method
hvap	86.61	kJ/mol	Joback Method
log10ws	-4.64		Crippen Method
logp	3.612		Crippen Method
mcvol	256.980	ml/mol	McGowan Method
pc	1541.49	kPa	Joback Method
rinpol	2403.00		NIST Webbook
rinpol	2403.00		NIST Webbook
tb	896.68	K	Joback Method
tc	1114.66	K	Joback Method
tf	510.87	K	Joback Method
vc	0.998	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	785.98	J/mol×K	896.68	Joback Method
cpg	798.66	J/mol×K	933.01	Joback Method
cpg	810.18	J/mol×K	969.34	Joback Method
cpg	820.54	J/mol×K	1005.67	Joback Method
cpg	829.77	J/mol×K	1042.00	Joback Method
cpg	837.88	J/mol×K	1078.33	Joback Method
cpg	844.91	J/mol×K	1114.66	Joback Method

Sources

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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U393273&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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