Glutaric acid, cyclohexylmethyl 4-acetylphenyl ester

Inchi: InChI=1S/C20H26O5/c1-15(21)17-10-12-18(13-11-17)25-20(23)9-5-8-19(22)24-14-16-6-
InchiKey: NNUDNEVJANJOIU-UHFFFAOYSA-N
Formula: C20H26O5
SMILES: CC(=O)c1ccc(OC(=O)CCCC(=O)OCC2CCCCC2)cc1
Mol. weight [g/mol]: 346.42

Physical Properties

Property code	Value	Unit	Source
gf	-352.01	kJ/mol	Joback Method
hf	-778.93	kJ/mol	Joback Method
hfus	40.22	kJ/mol	Joback Method
hvap	88.54	kJ/mol	Joback Method
log10ws	-5.15		Crippen Method
logp	4.088		Crippen Method
mcvol	274.490	ml/mol	McGowan Method
pc	1649.77	kPa	Joback Method
rinpol	2842.00		NIST Webbook
rinpol	2842.00		NIST Webbook
tb	914.66	K	Joback Method
tc	1140.45	K	Joback Method
tf	555.73	K	Joback Method
vc	1.034	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	887.87	J/mol×K	914.66	Joback Method
cpg	902.45	J/mol×K	952.29	Joback Method
cpg	915.48	J/mol×K	989.92	Joback Method
cpg	927.00	J/mol×K	1027.55	Joback Method
cpg	937.05	J/mol×K	1065.18	Joback Method
cpg	945.65	J/mol×K	1102.81	Joback Method
cpg	952.83	J/mol×K	1140.45	Joback Method
dvisc	0.0005492	Pa×s	555.73	Joback Method

dvisc	0.0003093	Pa×s	615.55	Joback Method
dvisc	0.0001929	Pa×s	675.37	Joback Method
dvisc	0.0001299	Pa×s	735.19	Joback Method
dvisc	0.0000928	Pa×s	795.02	Joback Method
dvisc	0.0000695	Pa×s	854.84	Joback Method
dvisc	0.0000541	Pa×s	914.66	Joback Method

Sources

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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U392036&Units=SI

Legend

cpg:	Ideal gas heat capacity
dvisc:	Dynamic viscosity
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