Glutaric acid, 4-acetylphenyl hexyl ester

Inchi: InChI=1S/C19H26O5/c1-3-4-5-6-14-23-18(21)8-7-9-19(22)24-17-12-10-16(11-13-17)15(2
InchiKey: ZBARMGGXXKGYED-UHFFFAOYSA-N
Formula: C19H26O5
SMILES: CCCCCCOC(=O)CCCC(=O)Oc1ccc(C(C)=O)cc1
Mol. weight [g/mol]: 334.41

Physical Properties

Property code	Value	Unit	Source
gf	-384.88	kJ/mol	Joback Method
hf	-812.61	kJ/mol	Joback Method
hfus	45.79	kJ/mol	Joback Method
hvap	85.88	kJ/mol	Joback Method
log10ws	-5.08		Crippen Method
logp	4.088		Crippen Method
mcvol	271.260	ml/mol	McGowan Method
pc	1512.85	kPa	Joback Method
rinpol	2666.00		NIST Webbook
tb	872.23	K	Joback Method
tc	1079.56	K	Joback Method
tf	537.08	K	Joback Method
vc	1.046	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	835.46	J/mol×K	872.23	Joback Method
cpg	894.84	J/mol×K	1045.00	Joback Method
cpg	885.18	J/mol×K	1010.45	Joback Method
cpg	874.44	J/mol×K	975.89	Joback Method
cpg	862.58	J/mol×K	941.34	Joback Method
cpg	849.59	J/mol×K	906.78	Joback Method
cpg	903.42	J/mol×K	1079.56	Joback Method
dvisc	0.0000605	Pa×s	872.23	Joback Method
dvisc	0.0000770	Pa×s	816.37	Joback Method

dvisc	0.0001014	Pa×s	760.51	Joback Method
dvisc	0.0001396	Pa×s	704.65	Joback Method
dvisc	0.0002030	Pa×s	648.80	Joback Method
dvisc	0.0003167	Pa×s	592.94	Joback Method
dvisc	0.0005421	Pa×s	537.08	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=U359267&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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