Glutaric acid, di(4-acetylphenyl) ester

Inchi: InChI=1S/C21H20O6/c1-14(22)16-6-10-18(11-7-16)26-20(24)4-3-5-21(25)27-19-12-8-17
InchiKey: ITYMCEKBTZGXGA-UHFFFAOYSA-N
Formula: C21H20O6
SMILES: CC(=O)c1ccc(OC(=O)CCCC(=O)Oc2ccc(C(C)=O)cc2)cc1
Mol. weight [g/mol]: 368.38

Physical Properties

Property code	Value	Unit	Source
gf	-394.18	kJ/mol	Joback Method
hf	-741.41	kJ/mol	Joback Method
hfus	46.22	kJ/mol	Joback Method
hvap	100.02	kJ/mol	Joback Method
log10ws	-5.49		Crippen Method
logp	3.773		Crippen Method
mcvol	277.250	ml/mol	McGowan Method
pc	1759.49	kPa	Joback Method
rinpol	3328.00		NIST Webbook
tb	1003.52	K	Joback Method
tc	1240.68	K	Joback Method
tf	648.49	K	Joback Method
vc	1.056	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	853.61	J/mol×K	1003.52	Joback Method
cpg	888.00	J/mol×K	1201.15	Joback Method
cpg	883.83	J/mol×K	1161.62	Joback Method
cpg	878.34	J/mol×K	1122.10	Joback Method
cpg	871.50	J/mol×K	1082.57	Joback Method
cpg	863.27	J/mol×K	1043.05	Joback Method
cpg	890.88	J/mol×K	1240.68	Joback Method
dvisc	0.0000454	Pa×s	1003.52	Joback Method
dvisc	0.0000565	Pa×s	944.35	Joback Method

dvisc	0.0000723	Pa×s	885.18	Joback Method
dvisc	0.0000958	Pa×s	826.00	Joback Method
dvisc	0.0001326	Pa×s	766.83	Joback Method
dvisc	0.0001938	Pa×s	707.66	Joback Method
dvisc	0.0003036	Pa×s	648.49	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=U359275&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