Glutaric acid, 4-acetylphenyl octyl ester

Inchi: InChI=1S/C21H30O5/c1-3-4-5-6-7-8-16-25-20(23)10-9-11-21(24)26-19-14-12-18(13-15-1
InchiKey: TVNCVLCLLVYTRA-UHFFFAOYSA-N
Formula: C21H30O5
SMILES: CCCCCCCCOC(=O)CCCC(=O)Oc1ccc(C(C)=O)cc1
Mol. weight [g/mol]: 362.46

Physical Properties

Property code	Value	Unit	Source
gf	-368.04	kJ/mol	Joback Method
hf	-853.89	kJ/mol	Joback Method
hfus	50.97	kJ/mol	Joback Method
hvap	90.34	kJ/mol	Joback Method
log10ws	-5.91		Crippen Method
logp	4.869		Crippen Method
mcvol	299.440	ml/mol	McGowan Method
pc	1309.90	kPa	Joback Method
rinpol	2867.00		NIST Webbook
rinpol	2867.00		NIST Webbook
tb	917.99	K	Joback Method
tc	1128.26	K	Joback Method
tf	559.62	K	Joback Method
vc	1.157	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	953.25	J/mol×K	917.99	Joback Method
cpg	967.76	J/mol×K	953.03	Joback Method
cpg	981.01	J/mol×K	988.08	Joback Method
cpg	993.02	J/mol×K	1023.12	Joback Method
cpg	1003.84	J/mol×K	1058.17	Joback Method
cpg	1013.48	J/mol×K	1093.21	Joback Method
cpg	1021.96	J/mol×K	1128.26	Joback Method
dvisc	0.0004391	Pa×s	559.62	Joback Method

dvisc	0.0002507	Pa×s	619.35	Joback Method
dvisc	0.0001580	Pa×s	679.08	Joback Method
dvisc	0.0001072	Pa×s	738.80	Joback Method
dvisc	0.0000772	Pa×s	798.53	Joback Method
dvisc	0.0000581	Pa×s	858.26	Joback Method
dvisc	0.0000454	Pa×s	917.99	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=U359269&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