Glutaric acid, 4-acetylphenyl butyl ester

Inchi: InChI=1S/C17H22O5/c1-3-4-12-21-16(19)6-5-7-17(20)22-15-10-8-14(9-11-15)13(2)18/h8
InchiKey: ZMAZUQXWYNZFNZ-UHFFFAOYSA-N
Formula: C17H22O5
SMILES: CCCCOC(=O)CCCC(=O)Oc1ccc(C(C)=O)cc1
Mol. weight [g/mol]: 306.35

Physical Properties

Property code	Value	Unit	Source
gf	-401.72	kJ/mol	Joback Method
hf	-771.33	kJ/mol	Joback Method
hfus	40.61	kJ/mol	Joback Method
hvap	81.43	kJ/mol	Joback Method
log10ws	-4.24		Crippen Method
logp	3.308		Crippen Method
mcvol	243.080	ml/mol	McGowan Method
pc	1766.90	kPa	Joback Method
rinpol	2456.00		NIST Webbook
rinpol	2456.00		NIST Webbook
tb	826.47	K	Joback Method
tc	1033.85	K	Joback Method
tf	514.54	K	Joback Method
vc	0.933	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	720.60	J/mol×K	826.47	Joback Method
cpg	778.68	J/mol×K	999.29	Joback Method
cpg	769.14	J/mol×K	964.72	Joback Method
cpg	758.57	J/mol×K	930.16	Joback Method
cpg	746.97	J/mol×K	895.60	Joback Method
cpg	734.32	J/mol×K	861.03	Joback Method
cpg	787.21	J/mol×K	1033.85	Joback Method
dvisc	0.0000799	Pa×s	826.47	Joback Method

dvisc	0.0001009	Pa×s	774.48	Joback Method
dvisc	0.0001318	Pa×s	722.49	Joback Method
dvisc	0.0001794	Pa×s	670.50	Joback Method
dvisc	0.0002573	Pa×s	618.52	Joback Method
dvisc	0.0003942	Pa×s	566.53	Joback Method
dvisc	0.0006584	Pa×s	514.54	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=U359264&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