Glutaric acid, 4-acetylphenyl isohexyl ester

Inchi: InChI=1S/C19H26O5/c1-14(2)6-5-13-23-18(21)7-4-8-19(22)24-17-11-9-16(10-12-17)15(3
InchiKey: SDAFEKZIKCGRFB-UHFFFAOYSA-N
Formula: C19H26O5
SMILES: CC(=O)c1ccc(OC(=O)CCCC(=O)OCCCC(C)C)cc1
Mol. weight [g/mol]: 334.41

Physical Properties

Property code	Value	Unit	Source
gf	-387.32	kJ/mol	Joback Method
hf	-817.89	kJ/mol	Joback Method
hfus	42.27	kJ/mol	Joback Method
hvap	85.50	kJ/mol	Joback Method
log10ws	-4.83		Crippen Method
logp	3.944		Crippen Method
mcvol	271.260	ml/mol	McGowan Method
pc	1522.31	kPa	Joback Method
rinpol	2625.00		NIST Webbook
tb	871.79	K	Joback Method
tc	1080.92	K	Joback Method
tf	522.08	K	Joback Method
vc	1.040	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	835.98	J/mol×K	871.79	Joback Method
cpg	850.22	J/mol×K	906.65	Joback Method
cpg	863.28	J/mol×K	941.50	Joback Method
cpg	875.17	J/mol×K	976.36	Joback Method
cpg	885.92	J/mol×K	1011.21	Joback Method
cpg	895.55	J/mol×K	1046.07	Joback Method
cpg	904.08	J/mol×K	1080.92	Joback Method
dvisc	0.0006006	Pa×s	522.08	Joback Method
dvisc	0.0003307	Pa×s	580.36	Joback Method

dvisc	0.0002030	Pa×s	638.65	Joback Method
dvisc	0.0001352	Pa×s	696.93	Joback Method
dvisc	0.0000959	Pa×s	755.22	Joback Method
dvisc	0.0000715	Pa×s	813.50	Joback Method
dvisc	0.0000554	Pa×s	871.79	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=U359266&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

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