

Glutaric acid, 4-acetylphenyl isobutyl ester

Inchi:	InChI=1S/C17H22O5/c1-12(2)11-21-16(19)5-4-6-17(20)22-15-9-7-14(8-10-15)13(3)18/h7
InchiKey:	XXODERYIRAVZRM-UHFFFAOYSA-N
Formula:	C17H22O5
SMILES:	CC(=O)c1ccc(OC(=O)CCCC(=O)OCC(C)C)cc1
Mol. weight [g/mol]:	306.35

Physical Properties

Property code	Value	Unit	Source
gf	-404.16	kJ/mol	Joback Method
hf	-776.61	kJ/mol	Joback Method
hfus	37.09	kJ/mol	Joback Method
hvap	81.04	kJ/mol	Joback Method
log10ws	-4.00		Crippen Method
logp	3.164		Crippen Method
mcvol	243.080	ml/mol	McGowan Method
pc	1778.84	kPa	Joback Method
rinqol	2407.00		NIST Webbook
tb	826.03	K	Joback Method
tc	1035.87	K	Joback Method
tf	499.54	K	Joback Method
vc	0.927	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	721.16	J/molxK	826.03	Joback Method
cpg	735.03	J/molxK	861.00	Joback Method
cpg	747.79	J/molxK	895.98	Joback Method
cpg	759.47	J/molxK	930.95	Joback Method
cpg	770.08	J/molxK	965.92	Joback Method
cpg	779.63	J/molxK	1000.89	Joback Method
cpg	788.14	J/molxK	1035.87	Joback Method
dvisc	0.0007347	Paxs	499.54	Joback Method
dvisc	0.0004142	Paxs	553.96	Joback Method

dvisc	0.0002588	Paxs	608.37	Joback Method
dvisc	0.0001746	Paxs	662.78	Joback Method
dvisc	0.0001251	Paxs	717.20	Joback Method
dvisc	0.0000939	Paxs	771.62	Joback Method
dvisc	0.0000732	Paxs	826.03	Joback Method

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
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=U359263&Units=SI

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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