

Glutaric acid, 4-acetylphenyl ethyl ester

Inchi:	InChI=1S/C15H18O5/c1-3-19-14(17)5-4-6-15(18)20-13-9-7-12(8-10-13)11(2)16/h7-10H,1
InchiKey:	XGMVYSWVAFPGGV-UHFFFAOYSA-N
Formula:	C15H18O5
SMILES:	CCOC(=O)CCCC(=O)Oc1ccc(C(C)=O)cc1
Mol. weight [g/mol]:	278.30

Physical Properties

Property code	Value	Unit	Source
gf	-418.56	kJ/mol	Joback Method
hf	-730.05	kJ/mol	Joback Method
hfus	35.43	kJ/mol	Joback Method
hvap	76.98	kJ/mol	Joback Method
log10ws	-3.40		Crippen Method
logp	2.528		Crippen Method
mcvol	214.900	ml/mol	McGowan Method
pc	2090.75	kPa	Joback Method
rinpol	2243.00		NIST Webbook
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tb	780.71	K	Joback Method
tc	990.74	K	Joback Method
tf	492.00	K	Joback Method
vc	0.822	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	609.26	J/molxK	780.71	Joback Method
cpg	665.32	J/molxK	955.73	Joback Method
cpg	656.04	J/molxK	920.73	Joback Method
cpg	645.81	J/molxK	885.72	Joback Method
cpg	634.60	J/molxK	850.72	Joback Method
cpg	622.42	J/molxK	815.71	Joback Method
cpg	673.64	J/molxK	990.74	Joback Method
dvisc	0.0001041	Paxs	780.71	Joback Method

dvisc	0.0001305	Paxs	732.59	Joback Method
dvisc	0.0001688	Paxs	684.47	Joback Method
dvisc	0.0002272	Paxs	636.36	Joback Method
dvisc	0.0003210	Paxs	588.24	Joback Method
dvisc	0.0004822	Paxs	540.12	Joback Method
dvisc	0.0007846	Paxs	492.00	Joback Method

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
Crippen Method:	https://www.cheméo.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=U359261&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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