

Glutaric acid, 2-methylpent-3-yl 4-acetylphenyl ester

Inchi: InChI=1S/C19H26O5/c1-5-17(13(2)3)24-19(22)8-6-7-18(21)23-16-11-9-15(10-12-16)14(4)
InchiKey: VYYIEDVGVBXKND-UHFFFAOYSA-N
Formula: C19H26O5
SMILES: CCC(OC(=O)CCCC(=O)Oc1ccc(C(C)=O)cc1)C(C)C
Mol. weight [g/mol]: 334.41

Physical Properties

Property code	Value	Unit	Source
gf	-389.76	kJ/mol	Joback Method
hf	-823.17	kJ/mol	Joback Method
hfus	38.74	kJ/mol	Joback Method
hvap	85.11	kJ/mol	Joback Method
log10ws	-4.95		Crippen Method
logp	3.943		Crippen Method
mcvol	271.260	ml/mol	McGowan Method
pc	1531.86	kPa	Joback Method
rinpol	2485.00		NIST Webbook
tb	871.35	K	Joback Method
tc	1082.44	K	Joback Method
tf	507.08	K	Joback Method
vc	1.034	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	836.51	J/mol×K	871.35	Joback Method
cpg	850.86	J/mol×K	906.53	Joback Method
cpg	863.99	J/mol×K	941.71	Joback Method
cpg	875.92	J/mol×K	976.89	Joback Method
cpg	886.69	J/mol×K	1012.07	Joback Method
cpg	896.29	J/mol×K	1047.25	Joback Method
cpg	904.77	J/mol×K	1082.44	Joback Method
dvisc	0.0006747	Pa×s	507.08	Joback Method
dvisc	0.0003480	Pa×s	567.79	Joback Method

dvisc	0.0002040	Pa×s	628.50	Joback Method
dvisc	0.0001313	Pa×s	689.22	Joback Method
dvisc	0.0000908	Pa×s	749.93	Joback Method
dvisc	0.0000664	Pa×s	810.64	Joback Method
dvisc	0.0000507	Pa×s	871.35	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=U392032&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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