

Glutaric acid, 2,6-dimethoxyphenyl pentyl ester

Inchi:	InChI=1S/C18H26O6/c1-4-5-6-13-23-16(19)11-8-12-17(20)24-18-14(21-2)9-7-10-15(18)2
InchiKey:	BVIOXSQLHIZIMZ-UHFFFAOYSA-N
Formula:	C18H26O6
SMILES:	CCCCOC(=O)CCCC(=O)Oc1c(OC)cccc1OC
Mol. weight [g/mol]:	338.40

Physical Properties

Property code	Value	Unit	Source
gf	-484.01	kJ/mol	Joback Method
hf	-955.30	kJ/mol	Joback Method
hfus	43.59	kJ/mol	Joback Method
hvap	82.39	kJ/mol	Joback Method
log10ws	-4.24		Crippen Method
logp	3.513		Crippen Method
mcvol	267.340	ml/mol	McGowan Method
pc	1494.19	kPa	Joback Method
rinqol	2501.00		NIST Webbook
tb	845.30	K	Joback Method
tc	1046.99	K	Joback Method
tf	532.86	K	Joback Method
vc	1.020	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	817.79	J/molxK	845.30	Joback Method
cpg	832.47	J/molxK	878.92	Joback Method
cpg	845.96	J/molxK	912.53	Joback Method
cpg	858.25	J/molxK	946.15	Joback Method
cpg	869.32	J/molxK	979.76	Joback Method
cpg	879.17	J/molxK	1013.38	Joback Method
cpg	887.77	J/molxK	1046.99	Joback Method
dvisc	0.0003135	Paxs	532.86	Joback Method
dvisc	0.0001926	Paxs	584.93	Joback Method

dvisc	0.0001281	Paxs	637.01	Joback Method
dvisc	0.0000906	Paxs	689.08	Joback Method
dvisc	0.0000673	Paxs	741.15	Joback Method
dvisc	0.0000520	Paxs	793.23	Joback Method
dvisc	0.0000415	Paxs	845.30	Joback Method

Sources

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=U358707&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.cheméo.com/doc/models/crippen_log10ws

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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