

Glutaric acid, 3-methylbut-2-yl 2,6-dimethoxyphenyl ester

Inchi:	InChI=1S/C18H26O6/c1-12(2)13(3)23-16(19)10-7-11-17(20)24-18-14(21-4)8-6-9-15(18)2
InchiKey:	JZJWJGRNFFZOBQ-UHFFFAOYSA-N
Formula:	C18H26O6
SMILES:	COc1cccc(OC)c1OC(=O)CCCC(=O)OC(C)C(C)C
Mol. weight [g/mol]:	338.40

Physical Properties

Property code	Value	Unit	Source
gf	-488.89	kJ/mol	Joback Method
hf	-965.86	kJ/mol	Joback Method
hfus	36.54	kJ/mol	Joback Method
hvap	81.62	kJ/mol	Joback Method
log10ws	-4.11		Crippen Method
logp	3.367		Crippen Method
mvol	267.340	ml/mol	McGowan Method
pc	1512.85	kPa	Joback Method
rinpol	2349.00		NIST Webbook
rinpol	2349.00		NIST Webbook
tb	844.42	K	Joback Method
tc	1049.87	K	Joback Method
tf	502.86	K	Joback Method
vc	1.008	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	818.86	J/molxK	844.42	Joback Method
cpg	880.80	J/molxK	1015.63	Joback Method
cpg	870.97	J/molxK	981.39	Joback Method
cpg	859.85	J/molxK	947.15	Joback Method
cpg	847.45	J/molxK	912.90	Joback Method
cpg	833.78	J/molxK	878.66	Joback Method
cpg	889.31	J/molxK	1049.87	Joback Method
dvisc	0.0000348	Paxs	844.42	Joback Method

dvisc	0.0000450	Paxs	787.49	Joback Method
dvisc	0.0000605	Paxs	730.57	Joback Method
dvisc	0.0000855	Paxs	673.64	Joback Method
dvisc	0.0001288	Paxs	616.71	Joback Method
dvisc	0.0002110	Paxs	559.79	Joback Method
dvisc	0.0003864	Paxs	502.86	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=U391999&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

Legend

cp_g:	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:	Log ₁₀ 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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