

Glutaric acid, butyl 2,6-dimethoxyphenyl ester

Inchi: InChI=1S/C17H24O6/c1-4-5-12-22-15(18)10-7-11-16(19)23-17-13(20-2)8-6-9-14(17)21-3
InchiKey: SNDCHVRMVVBTMN-UHFFFAOYSA-N
Formula: C17H24O6
SMILES: CCCCOC(=O)CCCC(=O)Oc1c(OC)cccc1OC
Mol. weight [g/mol]: 324.37

Physical Properties

Property code	Value	Unit	Source
gf	-492.43	kJ/mol	Joback Method
hf	-934.66	kJ/mol	Joback Method
hfus	41.00	kJ/mol	Joback Method
hvap	80.17	kJ/mol	Joback Method
log10ws	-3.82		Crippen Method
logp	3.123		Crippen Method
mcvol	253.250	ml/mol	McGowan Method
pc	1611.58	kPa	Joback Method
rinpol	2403.00		NIST Webbook
tb	822.42	K	Joback Method
tc	1023.77	K	Joback Method
tf	521.59	K	Joback Method
vc	0.964	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	760.08	J/molxK	822.42	Joback Method
cpg	821.14	J/molxK	990.21	Joback Method
cpg	811.23	J/molxK	956.65	Joback Method
cpg	800.16	J/molxK	923.09	Joback Method
cpg	787.93	J/molxK	889.54	Joback Method
cpg	774.57	J/molxK	855.98	Joback Method
cpg	829.86	J/molxK	1023.77	Joback Method
dvisc	0.0000476	Paxs	822.42	Joback Method
dvisc	0.0000595	Paxs	772.28	Joback Method

dvisc	0.0000767	Paxs	722.14	Joback Method
dvisc	0.0001026	Paxs	672.00	Joback Method
dvisc	0.0001440	Paxs	621.87	Joback Method
dvisc	0.0002144	Paxs	571.73	Joback Method
dvisc	0.0003446	Paxs	521.59	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=U358706&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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