

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

Inchi:	InChI=1S/C19H28O6/c1-6-14(13(2)3)24-17(20)11-8-12-18(21)25-19-15(22-4)9-7-10-16(
InchiKey:	SVDRNYGDYQQHQM-UHFFFAOYSA-N
Formula:	C19H28O6
SMILES:	CCC(OC(=O)CCCC(=O)Oc1c(OC)cccc1OC)C(C)C
Mol. weight [g/mol]:	352.42

Physical Properties

Property code	Value	Unit	Source
gf	-480.47	kJ/mol	Joback Method
hf	-986.50	kJ/mol	Joback Method
hfus	39.13	kJ/mol	Joback Method
hvap	83.84	kJ/mol	Joback Method
log10ws	-4.52		Crippen Method
logp	3.757		Crippen Method
mcvol	281.430	ml/mol	McGowan Method
pc	1405.90	kPa	Joback Method
rinpola	2429.00		NIST Webbook
tb	867.30	K	Joback Method
tc	1073.16	K	Joback Method
tf	514.13	K	Joback Method
vc	1.063	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	877.30	J/molxK	867.30	Joback Method
cpg	892.33	J/molxK	901.61	Joback Method
cpg	906.04	J/molxK	935.92	Joback Method
cpg	918.41	J/molxK	970.23	Joback Method
cpg	929.45	J/molxK	1004.54	Joback Method
cpg	939.12	J/molxK	1038.85	Joback Method
cpg	947.44	J/molxK	1073.16	Joback Method
dvisc	0.0003477	Paxs	514.13	Joback Method
dvisc	0.0001876	Paxs	572.99	Joback Method

dvisc	0.0001136	Paxs	631.85	Joback Method
dvisc	0.0000749	Paxs	690.71	Joback Method
dvisc	0.0000527	Paxs	749.58	Joback Method
dvisc	0.0000391	Paxs	808.44	Joback Method
dvisc	0.0000302	Paxs	867.30	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U392000&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Joback Method:	https://en.wikipedia.org/wiki/Joback_method

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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