Glutaric acid, 2-ethylhexyl 2,6-dimethoxyphenyl ester

Inchi: InChI=1S/C21H32O6/c1-5-7-10-16(6-2)15-26-19(22)13-9-14-20(23)27-21-17(24-3)11-8-1

InchiKey: CELNTRRARCEJCL-UHFFFAOYSA-N

Formula: C21H32O6

SMILES: CCCCC(CC)COC(=O)CCCC(=O)Oc1c(OC)cccc1OC

Mol. weight [g/mol]: 380.48

Physical Properties

Property code	Value	Unit	Source
gf	-461.19	kJ/mol	Joback Method
hf	-1022.50	kJ/mol	Joback Method
hfus	47.84	kJ/mol	Joback Method
hvap	88.68	kJ/mol	Joback Method
log10ws	-5.25		Crippen Method
logp	4.539		Crippen Method
mcvol	309.610	ml/mol	McGowan Method
pc	1216.59	kPa	Joback Method
rinpol	2671.00		NIST Webbook
rinpol	2671.00		NIST Webbook
tb	913.50	K	Joback Method
tc	1121.52	K	Joback Method
tf	551.67	K	Joback Method
vc	1.181	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	995.65	J/mol×K	913.50	Joback Method
cpg	1056.76	J/mol×K	1086.85	Joback Method
cpg	1047.46	J/mol×K	1052.18	Joback Method
cpg	1036.70	J/mol×K	1017.51	Joback Method
cpg	1024.47	J/mol×K	982.84	Joback Method
cpg	1010.79	J/mol×K	948.17	Joback Method
cpg	1064.58	J/mol×K	1121.52	Joback Method
dvisc	0.0000246	Pa×s	913.50	Joback Method

dvisc	0.0000316	Pa×s	853.19	Joback Method
dvisc	0.0000422	Pa×s	792.89	Joback Method
dvisc	0.0000591	Pa×s	732.59	Joback Method
dvisc	0.0000878	Pa×s	672.28	Joback Method
dvisc	0.0001411	Pa×s	611.98	Joback Method
dvisc	0.0002517	Pa×s	551.67	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U392006&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
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

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