Glutaric acid, di(5-methoxy-3-phenylpentyl) ester

Inchi: InChI=1S/C29H40O6/c1-32-20-16-26(24-10-5-3-6-11-24)18-22-34-28(30)14-9-15-29(31)35-23-19-27(21-17-33-2)25-12-7-4-8-13-25/h3-8,10-13,26-27H,9,14-23H2,1-2H3

InchiKey: RDKOKXBIOLKPQV-UHFFFAOYSA-N

Formula: C29H40O6

SMILES: COCCC(CCOC(=O)CCCC(=O)OCCC(CCOC)c1ccccc1)c1ccccc1

Mol. weight [g/mol]: 484.62

Physical Properties

Property code	Value	Unit	Source
gf	-264.60	kJ/mol	Joback Method
hf	-933.43	kJ/mol	Joback Method
hfus	59.85	kJ/mol	Joback Method
hvap	107.06	kJ/mol	Joback Method
log10ws	-5.99		Crippen Method
logp	5.664		Crippen Method
mcvol	398.570	ml/mol	McGowan Method
pc	937.49	kPa	Joback Method
rinpol	3615.00		NIST Webbook
rinpol	3615.00		NIST Webbook
tb	1112.82	K	Joback Method
tc	1365.10	K	Joback Method
tf	628.21	K	Joback Method
vc	1.516	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1374.88	J/mol×K	1112.82	Joback Method
cpg	1386.73	J/mol×K	1154.87	Joback Method
cpg	1396.33	J/mol×K	1196.91	Joback Method
cpg	1403.76	J/mol×K	1238.96	Joback Method
cpg	1409.09	J/mol×K	1281.01	Joback Method
cpg	1412.37	J/mol×K	1323.06	Joback Method
cpg	1413.67	J/mol×K	1365.10	Joback Method
dvisc	0.0001136	Pa×s	628.21	Joback Method

dvisc	0.0000534	Pa×s	708.98	Joback Method
dvisc	0.0000293	Pa×s	789.75	Joback Method
dvisc	0.0000180	Pa×s	870.51	Joback Method
dvisc	0.0000120	Pa×s	951.28	Joback Method
dvisc	0.0000085	Pa×s	1032.05	Joback Method
dvisc	0.0000063	Pa×s	1112.82	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=U359540&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.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