Glutaric acid, decyl 5-methoxy-3-phenylpentyl ester

Inchi: InChI=1S/C27H44O5/c1-3-4-5-6-7-8-9-13-21-31-26(28)17-14-18-27(29)32-23-20-25(19-2

InchiKey: LYEBXQLKHBXISI-UHFFFAOYSA-N

Formula: C27H44O5

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

Mol. weight [g/mol]: 448.64

Physical Properties

Property code	Value	Unit	Source
gf	-286.41	kJ/mol	Joback Method
hf	-991.18	kJ/mol	Joback Method
hfus	62.97	kJ/mol	Joback Method
hvap	98.31	kJ/mol	Joback Method
log10ws	-7.00		Crippen Method
logp	6.594		Crippen Method
mcvol	388.280	ml/mol	McGowan Method
pc	867.09	kPa	Joback Method
rinpol	3228.00		NIST Webbook
tb	1018.40	K	Joback Method
tc	1250.07	K	Joback Method
tf	572.02	K	Joback Method
vc	1.500	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1336.63	J/mol×K	1018.40	Joback Method
cpg	1403.80	J/mol×K	1211.46	Joback Method
cpg	1393.88	J/mol×K	1172.85	Joback Method
cpg	1382.26	J/mol×K	1134.24	Joback Method
cpg	1368.88	J/mol×K	1095.62	Joback Method
cpg	1353.69	J/mol×K	1057.01	Joback Method
cpg	1412.06	J/mol×K	1250.07	Joback Method
dvisc	0.0000127	Pa×s	1018.40	Joback Method
dvisc	0.0000170	Pa×s	944.00	Joback Method

dvisc	0.0000240	Pa×s	869.61	Joback Method
dvisc	0.0000361	Pa×s	795.21	Joback Method
dvisc	0.0000589	Pa×s	720.81	Joback Method
dvisc	0.0001078	Pa×s	646.42	Joback Method
dvisc	0.0002308	Pa×s	572.02	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U359536&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

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