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

Inchi: InChI=1S/C28H46O5/c1-3-4-5-6-7-8-9-10-14-22-32-27(29)18-15-19-28(30)33-24-21-26(2

InchiKey: CIDNCBYKGKFIQP-UHFFFAOYSA-N

Formula: C28H46O5

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

Mol. weight [g/mol]: 462.66

Physical Properties

Property code	Value	Unit	Source
gf	-277.99	kJ/mol	Joback Method
hf	-1011.82	kJ/mol	Joback Method
hfus	65.56	kJ/mol	Joback Method
hvap	100.53	kJ/mol	Joback Method
log10ws	-7.42		Crippen Method
logp	6.984		Crippen Method
mcvol	402.370	ml/mol	McGowan Method
pc	820.07	kPa	Joback Method
rinpol	3334.00		NIST Webbook
rinpol	3334.00		NIST Webbook
tb	1041.28	K	Joback Method
tc	1281.47	K	Joback Method
tf	583.29	K	Joback Method
vc	1.556	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1399.43	J/mol×K	1041.28	Joback Method
cpg	1466.31	J/mol×K	1241.44	Joback Method
cpg	1456.72	J/mol×K	1201.41	Joback Method
cpg	1445.30	J/mol×K	1161.37	Joback Method
cpg	1431.99	J/mol×K	1121.34	Joback Method
cpg	1416.72	J/mol×K	1081.31	Joback Method
cpg	1474.14	J/mol×K	1281.47	Joback Method
dvisc	0.0000108	Pa×s	1041.28	Joback Method

dvisc	0.0000146	Pa×s	964.95	Joback Method
dvisc	0.0000206	Pa×s	888.62	Joback Method
dvisc	0.0000310	Pa×s	812.28	Joback Method
dvisc	0.0000508	Pa×s	735.95	Joback Method
dvisc	0.0000935	Pa×s	659.62	Joback Method
dvisc	0.0002017	Pa×s	583.29	Joback Method

Sources

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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U359537&Units=SI

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