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

Inchi: InChI=1S/C30H50O5/c1-3-4-5-6-7-8-9-10-11-12-16-24-34-29(31)20-17-21-30(32)35-26-2

InchiKey: CRXCPVAZNRLLFO-UHFFFAOYSA-N

Formula: C30H50O5

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

Mol. weight [g/mol]: 490.71

Physical Properties

Property code	Value	Unit	Source
gf	-261.15	kJ/mol	Joback Method
hf	-1053.10	kJ/mol	Joback Method
hfus	70.74	kJ/mol	Joback Method
hvap	104.98	kJ/mol	Joback Method
log10ws	-8.26		Crippen Method
logp	7.764		Crippen Method
mcvol	430.550	ml/mol	McGowan Method
pc	736.82	kPa	Joback Method
rinpol	3554.00		NIST Webbook
tb	1087.04	K	Joback Method
tc	1348.32	K	Joback Method
tf	605.83	K	Joback Method
vc	1.667	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1525.75	J/mol×K	1087.04	Joback Method
cpg	1543.55	J/mol×K	1130.59	Joback Method
cpg	1558.94	J/mol×K	1174.13	Joback Method
cpg	1572.03	J/mol×K	1217.68	Joback Method
cpg	1582.89	J/mol×K	1261.23	Joback Method
cpg	1591.64	J/mol×K	1304.77	Joback Method
cpg	1598.36	J/mol×K	1348.32	Joback Method
dvisc	0.0001531	Pa×s	605.83	Joback Method
dvisc	0.0000699	Pa×s	686.03	Joback Method

dvisc	0.0000376	Pa×s	766.23	Joback Method
dvisc	0.0000227	Pa×s	846.43	Joback Method
dvisc	0.0000150	Pa×s	926.64	Joback Method
dvisc	0.0000106	Pa×s	1006.84	Joback Method
dvisc	0.0000079	Pa×s	1087.04	Joback Method

Sources

McGowan Method: http://link.springer.com/article/10.1007/BF02311772
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=U359539&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