Glutaric acid, phenethyl tridecyl ester

Inchi: InChI=1S/C26H42O4/c1-2-3-4-5-6-7-8-9-10-11-15-22-29-25(27)19-16-20-26(28)30-23-21
InchiKey: LQNCMCBRPCCSRL-UHFFFAOYSA-N
Formula: C26H42O4
SMILES: CCCCCCCCCCCCCOC(=O)CCCC(=O)OCCc1ccccc1
Mol. weight [g/mol]: 418.61

Physical Properties

Property code	Value	Unit	Source
gf	-187.39	kJ/mol	Joback Method
hf	-833.04	kJ/mol	Joback Method
hfus	62.71	kJ/mol	Joback Method
hvap	94.06	kJ/mol	Joback Method
log10ws	-7.53		Crippen Method
logp	6.797		Crippen Method
mcvol	368.320	ml/mol	McGowan Method
pc	923.30	kPa	Joback Method
rinpol	3168.00		NIST Webbook
rinpol	3168.00		NIST Webbook
tb	973.54	K	Joback Method
tc	1192.35	K	Joback Method
tf	553.52	K	Joback Method
vc	1.431	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1244.21	J/mol×K	973.54	Joback Method
cpg	1261.91	J/mol×K	1010.01	Joback Method
cpg	1278.10	J/mol×K	1046.48	Joback Method
cpg	1292.83	J/mol×K	1082.94	Joback Method
cpg	1306.17	J/mol×K	1119.41	Joback Method
cpg	1318.16	J/mol×K	1155.88	Joback Method
cpg	1328.87	J/mol×K	1192.35	Joback Method
dvisc	0.0003484	Pa×s	553.52	Joback Method

dvisc	0.0001703	Pa×s	623.52	Joback Method
dvisc	0.0000962	Pa×s	693.53	Joback Method
dvisc	0.0000603	Pa×s	763.53	Joback Method
dvisc	0.0000409	Pa×s	833.53	Joback Method
dvisc	0.0000295	Pa×s	903.54	Joback Method
dvisc	0.0000223	Pa×s	973.54	Joback Method

Sources

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=U358689&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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