Glutaric acid, 1-phenylpropyl tetradecyl ester

Inchi: InChI=1S/C28H46O4/c1-3-5-6-7-8-9-10-11-12-13-14-18-24-31-27(29)22-19-23-28(30)32
InchiKey: SOVLZKTXBHEFSA-UHFFFAOYSA-N
Formula: C28H46O4
SMILES: CCCCCCCCCCCCCCOC(=O)CCCC(=O)OC(CC)c1ccccc1
Mol. weight [g/mol]: 446.66

Physical Properties

Property code	Value	Unit	Source
gf	-172.99	kJ/mol	Joback Method
hf	-879.60	kJ/mol	Joback Method
hfus	64.37	kJ/mol	Joback Method
hvap	98.12	kJ/mol	Joback Method
log10ws	-8.83		Crippen Method
logp	8.095		Crippen Method
mcvol	396.500	ml/mol	McGowan Method
pc	828.11	kPa	Joback Method
rinpol	3218.00		NIST Webbook
tb	1018.86	K	Joback Method
tc	1250.94	K	Joback Method
tf	561.06	K	Joback Method
vc	1.538	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1370.47	J/mol×K	1018.86	Joback Method
cpg	1445.12	J/mol×K	1212.26	Joback Method
cpg	1433.35	J/mol×K	1173.58	Joback Method
cpg	1420.07	J/mol×K	1134.90	Joback Method
cpg	1405.22	J/mol×K	1096.22	Joback Method
cpg	1388.71	J/mol×K	1057.54	Joback Method
cpg	1455.46	J/mol×K	1250.94	Joback Method
dvisc	0.0000148	Pa×s	1018.86	Joback Method
dvisc	0.0000200	Pa×s	942.56	Joback Method

dvisc	0.0000284	Pa×s	866.26	Joback Method
dvisc	0.0000431	Pa×s	789.96	Joback Method
dvisc	0.0000717	Pa×s	713.66	Joback Method
dvisc	0.0001346	Pa×s	637.36	Joback Method
dvisc	0.0002999	Pa×s	561.06	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=U358960&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