Glutaric acid, hexadecyl 1-phenylpropyl ester

Inchi: InChI=1S/C30H50O4/c1-3-5-6-7-8-9-10-11-12-13-14-15-16-20-26-33-29(31)24-21-25-30
InchiKey: SOIKDHSNUYFAAD-UHFFFAOYSA-N
Formula: C30H50O4
SMILES: CCCCCCCCCCCCCCCCOC(=O)CCCC(=O)OC(CC)c1ccccc1
Mol. weight [g/mol]: 474.72

Physical Properties

Property code	Value	Unit	Source
gf	-156.15	kJ/mol	Joback Method
hf	-920.88	kJ/mol	Joback Method
hfus	69.55	kJ/mol	Joback Method
hvap	102.57	kJ/mol	Joback Method
log10ws	-9.67		Crippen Method
logp	8.876		Crippen Method
mcvol	424.680	ml/mol	McGowan Method
pc	743.67	kPa	Joback Method
rinpol	3431.00		NIST Webbook
rinpol	3431.00		NIST Webbook
tb	1064.62	K	Joback Method
tc	1315.33	K	Joback Method
tf	583.60	K	Joback Method
vc	1.649	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1497.72	J/mol×K	1064.62	Joback Method
cpg	1573.73	J/mol×K	1273.55	Joback Method
cpg	1562.13	J/mol×K	1231.76	Joback Method
cpg	1548.83	J/mol×K	1189.98	Joback Method
cpg	1533.74	J/mol×K	1148.19	Joback Method
cpg	1516.73	J/mol×K	1106.41	Joback Method
cpg	1583.75	J/mol×K	1315.33	Joback Method
dvisc	0.0000108	Pa×s	1064.62	Joback Method

dvisc	0.0000146	Pa×s	984.45	Joback Method
dvisc	0.0000208	Pa×s	904.28	Joback Method
dvisc	0.0000318	Pa×s	824.11	Joback Method
dvisc	0.0000532	Pa×s	743.94	Joback Method
dvisc	0.0001009	Pa×s	663.77	Joback Method
dvisc	0.0002283	Pa×s	583.60	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U358962&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
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

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