Glutaric acid, hexadecyl 4-methoxyphenyl ester

Inchi: InChI=1S/C28H46O5/c1-3-4-5-6-7-8-9-10-11-12-13-14-15-16-24-32-27(29)18-17-19-28(3

InchiKey: HIQNGTKFHGWBJK-UHFFFAOYSA-N

Formula: C28H46O5

SMILES: CCCCCCCCCCCCCCCCOC(=O)CCCC(=O)Oc1ccc(OC)cc1

Mol. weight [g/mol]: 462.66

Physical Properties

Property code	Value	Unit	Source
gf	-285.18	kJ/mol	Joback Method
hf	-1018.01	kJ/mol	Joback Method
hfus	68.69	kJ/mol	Joback Method
hvap	101.58	kJ/mol	Joback Method
log10ws	-8.72		Crippen Method
logp	7.795		Crippen Method
mcvol	402.370	ml/mol	McGowan Method
pc	809.37	kPa	Joback Method
rinpol	3564.00		NIST Webbook
tb	1046.70	K	Joback Method
tc	1290.03	K	Joback Method
tf	610.81	K	Joback Method
vc	1.562	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1398.39	J/mol×K	1046.70	Joback Method
cpg	1464.35	J/mol×K	1249.48	Joback Method
cpg	1455.12	J/mol×K	1208.92	Joback Method
cpg	1443.96	J/mol×K	1168.37	Joback Method
cpg	1430.83	J/mol×K	1127.81	Joback Method
cpg	1415.66	J/mol×K	1087.26	Joback Method
cpg	1471.71	J/mol×K	1290.03	Joback Method
dvisc	0.0000123	Pa×s	1046.70	Joback Method
dvisc	0.0000161	Pa×s	974.05	Joback Method

dvisc	0.0000220	Pa×s	901.40	Joback Method
dvisc	0.0000318	Pa×s	828.75	Joback Method
dvisc	0.0000493	Pa×s	756.11	Joback Method
dvisc	0.0000840	Pa×s	683.46	Joback Method
dvisc	0.0001623	Pa×s	610.81	Joback Method

Sources

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=U358750&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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