Glutaric acid, hexadecyl 3-methoxybenzyl ester

Inchi: InChI=1S/C29H48O5/c1-3-4-5-6-7-8-9-10-11-12-13-14-15-16-23-33-28(30)21-18-22-29(3

InchiKey: VIFXKTBPMZHAID-UHFFFAOYSA-N

Formula: C29H48O5

SMILES: CCCCCCCCCCCCCCCCOC(=O)CCCC(=O)OCc1cccc(OC)c1

Mol. weight [g/mol]: 476.69

Physical Properties

Property code	Value	Unit	Source
gf	-276.76	kJ/mol	Joback Method
hf	-1038.65	kJ/mol	Joback Method
hfus	71.28	kJ/mol	Joback Method
hvap	103.81	kJ/mol	Joback Method
log10ws	-8.99		Crippen Method
logp	7.933		Crippen Method
mcvol	416.460	ml/mol	McGowan Method
pc	766.91	kPa	Joback Method
rinpol	3561.00		NIST Webbook
tb	1069.58	K	Joback Method
tc	1323.36	K	Joback Method
tf	622.08	K	Joback Method
vc	1.617	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1461.42	J/mol×K	1069.58	Joback Method
cpg	1526.78	J/mol×K	1281.06	Joback Method
cpg	1518.01	J/mol×K	1238.77	Joback Method
cpg	1507.16	J/mol×K	1196.47	Joback Method
cpg	1494.16	J/mol×K	1154.17	Joback Method
cpg	1478.94	J/mol×K	1111.88	Joback Method
cpg	1533.52	J/mol×K	1323.36	Joback Method
dvisc	0.0000105	Pa×s	1069.58	Joback Method
dvisc	0.0000137	Pa×s	995.00	Joback Method

dvisc	0.0000189	Pa×s	920.41	Joback Method
dvisc	0.0000274	Pa×s	845.83	Joback Method
dvisc	0.0000426	Pa×s	771.25	Joback Method
dvisc	0.0000731	Pa×s	696.66	Joback Method
dvisc	0.0001425	Pa×s	622.08	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=U377201&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