Glutaric acid, cyclohexylmethyl octadecyl ester

Inchi: InChI=1S/C30H56O4/c1-2-3-4-5-6-7-8-9-10-11-12-13-14-15-16-20-26-33-29(31)24-21-25

InchiKey: QVHOSSCSDOEURS-UHFFFAOYSA-N

Formula: C30H56O4

SMILES: CCCCCCCCCCCCCCCCCCCCOC(=O)CCCC(=O)OCC1CCCCC1

Mol. weight [g/mol]: 480.76

Physical Properties

Property code	Value	Unit	Source
gf	-241.67	kJ/mol	Joback Method
hf	-1097.81	kJ/mol	Joback Method
hfus	70.86	kJ/mol	Joback Method
hvap	101.11	kJ/mol	Joback Method
log10ws	-9.76		Crippen Method
logp	9.085		Crippen Method
mcvol	437.580	ml/mol	McGowan Method
pc	692.16	kPa	Joback Method
rinpol	3502.00		NIST Webbook
rinpol	3502.00		NIST Webbook
tb	1057.93	K	Joback Method
tc	1311.35	K	Joback Method
tf	579.56	K	Joback Method
vc	1.696	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1600.46	J/mol×K	1057.93	Joback Method
cpg	1621.72	J/mol×K	1100.17	Joback Method
cpg	1640.56	J/mol×K	1142.40	Joback Method
cpg	1657.09	J/mol×K	1184.64	Joback Method
cpg	1671.40	J/mol×K	1226.88	Joback Method
cpg	1683.60	J/mol×K	1269.12	Joback Method
cpg	1693.79	J/mol×K	1311.35	Joback Method
dvisc	0.0002637	Pa×s	579.56	Joback Method

dvisc	0.0001146	Pa×s	659.29	Joback Method
dvisc	0.0000596	Pa×s	739.02	Joback Method
dvisc	0.0000352	Pa×s	818.74	Joback Method
dvisc	0.0000228	Pa×s	898.47	Joback Method
dvisc	0.0000159	Pa×s	978.20	Joback Method
dvisc	0.0000117	Pa×s	1057.93	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=U391649&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