Glutaric acid, cyclohexylmethyl heptadecyl ester

Inchi: InChI=1S/C29H54O4/c1-2-3-4-5-6-7-8-9-10-11-12-13-14-15-19-25-32-28(30)23-20-24-29

InchiKey: IKKAWKVDRLQJQE-UHFFFAOYSA-N

Formula: C29H54O4

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

Mol. weight [g/mol]: 466.74

Physical Properties

Property code	Value	Unit	Source
gf	-250.09	kJ/mol	Joback Method
hf	-1077.17	kJ/mol	Joback Method
hfus	68.28	kJ/mol	Joback Method
hvap	98.89	kJ/mol	Joback Method
log10ws	-9.34		Crippen Method
logp	8.695		Crippen Method
mcvol	423.490	ml/mol	McGowan Method
pc	728.49	kPa	Joback Method
rinpol	3359.00		NIST Webbook
rinpol	3359.00		NIST Webbook
tb	1035.05	K	Joback Method
tc	1277.56	K	Joback Method
tf	568.29	K	Joback Method
vc	1.641	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1535.56	J/mol×K	1035.05	Joback Method
cpg	1556.44	J/mol×K	1075.47	Joback Method
cpg	1575.11	J/mol×K	1115.89	Joback Method
cpg	1591.65	J/mol×K	1156.30	Joback Method
cpg	1606.14	J/mol×K	1196.72	Joback Method
cpg	1618.66	J/mol×K	1237.14	Joback Method
cpg	1629.31	J/mol×K	1277.56	Joback Method
dvisc	0.0003035	Pa×s	568.29	Joback Method

dvisc	0.0001328	Pa×s	646.08	Joback Method
dvisc	0.0000694	Pa×s	723.88	Joback Method
dvisc	0.0000411	Pa×s	801.67	Joback Method
dvisc	0.0000267	Pa×s	879.46	Joback Method
dvisc	0.0000186	Pa×s	957.26	Joback Method
dvisc	0.0000137	Pa×s	1035.05	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U393702&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

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