Glutaric acid, cyclohexylmethyl 3-methylbutyl ester

Inchi: InChI=1S/C17H30O4/c1-14(2)11-12-20-16(18)9-6-10-17(19)21-13-15-7-4-3-5-8-15/h14-1

InchiKey: VVDIZUUQOWIXSW-UHFFFAOYSA-N

Formula: C17H30O4

SMILES: CC(C)CCOC(=O)CCCC(=O)OCC1CCCCC1

Mol. weight [g/mol]: 298.42

Physical Properties

Property code	Value	Unit	Source
gf	-353.57	kJ/mol	Joback Method
hf	-834.77	kJ/mol	Joback Method
hfus	33.67	kJ/mol	Joback Method
hvap	71.79	kJ/mol	Joback Method
log10ws	-4.08		Crippen Method
logp	3.870		Crippen Method
mcvol	254.410	ml/mol	McGowan Method
pc	1543.92	kPa	Joback Method
rinpol	2246.00		NIST Webbook
rinpol	2246.00		NIST Webbook
tb	760.05	K	Joback Method
tc	957.86	K	Joback Method
tf	418.05	K	Joback Method
vc	0.963	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	787.48	J/mol×K	760.05	Joback Method
cpg	869.31	J/mol×K	924.89	Joback Method
cpg	855.29	J/mol×K	891.92	Joback Method
cpg	840.11	J/mol×K	858.95	Joback Method
cpg	823.76	J/mol×K	825.99	Joback Method
cpg	806.22	J/mol×K	793.02	Joback Method
cpg	882.19	J/mol×K	957.86	Joback Method
dvisc	0.0000777	Pa×s	760.05	Joback Method

dvisc	0.0001049	Pa×s	703.05	Joback Method
dvisc	0.0001492	Pa×s	646.05	Joback Method
dvisc	0.0002273	Pa×s	589.05	Joback Method
dvisc	0.0003788	Pa×s	532.05	Joback Method
dvisc	0.0007139	Pa×s	475.05	Joback Method
dvisc	0.0015992	Pa×s	418.05	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U391440&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