Glutaric acid, cyclopentyl cyclohexylmethyl ester

Inchi: InChI=1S/C17H28O4/c18-16(20-13-14-7-2-1-3-8-14)11-6-12-17(19)21-15-9-4-5-10-15/h1

InchiKey: MORKDYWYDVLJFS-UHFFFAOYSA-N

Formula: C17H28O4

SMILES: O=C(CCCC(=O)OC1CCCC1)OCC1CCCCC1

Mol. weight [g/mol]: 296.40

Physical Properties

Property code	Value	Unit	Source
gf	-314.58	kJ/mol	Joback Method
hf	-769.01	kJ/mol	Joback Method
hfus	31.13	kJ/mol	Joback Method
hvap	72.43	kJ/mol	Joback Method
log10ws	-4.32		Crippen Method
logp	3.766		Crippen Method
mcvol	243.550	ml/mol	McGowan Method
pc	1775.84	kPa	Joback Method
rinpol	2208.00		NIST Webbook
rinpol	2208.00		NIST Webbook
tb	775.77	K	Joback Method
tc	990.32	K	Joback Method
tf	443.95	K	Joback Method
vc	0.909	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	779.26	J/mol×K	775.77	Joback Method
cpg	863.82	J/mol×K	954.56	Joback Method
cpg	849.73	J/mol×K	918.80	Joback Method
cpg	834.26	J/mol×K	883.04	Joback Method
cpg	817.38	J/mol×K	847.29	Joback Method
cpg	799.05	J/mol×K	811.53	Joback Method
cpg	876.56	J/mol×K	990.32	Joback Method
dvisc	0.0001234	Pa×s	775.77	Joback Method

dvisc	0.0001609	Pa×s	720.47	Joback Method
dvisc	0.0002194	Pa×s	665.16	Joback Method
dvisc	0.0003162	Pa×s	609.86	Joback Method
dvisc	0.0004904	Pa×s	554.56	Joback Method
dvisc	0.0008380	Pa×s	499.25	Joback Method
dvisc	0.0016368	Pa×s	443.95	Joback Method

Sources

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
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U405395&Units=SI

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

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