

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
mvol	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	m ³ /kmol	Joback Method

Temperature Dependent Properties

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

dvisc	0.0001609	Paxs	720.47	Joback Method
dvisc	0.0002194	Paxs	665.16	Joback Method
dvisc	0.0003162	Paxs	609.86	Joback Method
dvisc	0.0004904	Paxs	554.56	Joback Method
dvisc	0.0008380	Paxs	499.25	Joback Method
dvisc	0.0016368	Paxs	443.95	Joback Method

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
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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