Glutaric acid, 1-cyclopentylethyl cyclohexylmethyl ester

Inchi: InChI=1S/C19H32O4/c1-15(17-10-5-6-11-17)23-19(21)13-7-12-18(20)22-14-16-8-3-2-4-9

InchiKey: SOGGQQDJRAWKGI-UHFFFAOYSA-N

Formula: C19H32O4

SMILES: CC(OC(=O)CCCC(=O)OCC1CCCCC1)C1CCCC1

Mol. weight [g/mol]: 324.45

Physical Properties

Property code	Value	Unit	Source
gf	-300.18	kJ/mol	Joback Method
hf	-815.57	kJ/mol	Joback Method
hfus	32.79	kJ/mol	Joback Method
hvap	76.50	kJ/mol	Joback Method
log10ws	-4.92		Crippen Method
logp	4.402		Crippen Method
mcvol	271.730	ml/mol	McGowan Method
pc	1529.46	kPa	Joback Method
rinpol	2334.00		NIST Webbook
rinpol	2334.00		NIST Webbook
tb	821.09	K	Joback Method
tc	1034.67	K	Joback Method
tf	451.49	K	Joback Method
vc	1.016	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	898.85	J/mol×K	821.09	Joback Method
cpg	918.75	J/mol×K	856.69	Joback Method
cpg	937.09	J/mol×K	892.28	Joback Method
cpg	953.91	J/mol×K	927.88	Joback Method
cpg	969.26	J/mol×K	963.47	Joback Method
cpg	983.16	J/mol×K	999.07	Joback Method
cpg	995.65	J/mol×K	1034.67	Joback Method
dvisc	0.0015700	Pa×s	451.49	Joback Method

dvisc	0.0007244	Pa×s	513.09	Joback Method
dvisc	0.0003945	Pa×s	574.69	Joback Method
dvisc	0.0002417	Pa×s	636.29	Joback Method
dvisc	0.0001614	Pa×s	697.89	Joback Method
dvisc	0.0001151	Pa×s	759.49	Joback Method
dvisc	0.0000864	Pa×s	821.09	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=U405464&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