Glutaric acid, 1-cyclopentylethyl 2-methylpent-3-yl ester

Inchi: InChI=1S/C18H32O4/c1-5-16(13(2)3)22-18(20)12-8-11-17(19)21-14(4)15-9-6-7-10-15/h1

InchiKey: FQSAFYUOADMTLL-UHFFFAOYSA-N

Formula: C18H32O4

SMILES: CCC(OC(=O)CCCC(=O)OC(C)C1CCCC1)C(C)C

Mol. weight [g/mol]: 312.44

Physical Properties

Property code	Value	Unit	Source
gf	-337.93	kJ/mol	Joback Method
hf	-859.81	kJ/mol	Joback Method
hfus	31.32	kJ/mol	Joback Method
hvap	73.07	kJ/mol	Joback Method
log10ws	-4.72		Crippen Method
logp	4.256		Crippen Method
mcvol	268.500	ml/mol	McGowan Method
pc	1423.99	kPa	Joback Method
rinpol	2000.00		NIST Webbook
rinpol	2000.00		NIST Webbook
tb	777.78	K	Joback Method
tc	975.46	K	Joback Method
tf	402.84	K	Joback Method
vc	1.014	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	843.47	J/mol×K	777.78	Joback Method
cpg	862.32	J/mol×K	810.73	Joback Method
cpg	879.96	J/mol×K	843.67	Joback Method
cpg	896.42	J/mol×K	876.62	Joback Method
cpg	911.71	J/mol×K	909.57	Joback Method
cpg	925.86	J/mol×K	942.51	Joback Method
cpg	938.91	J/mol×K	975.46	Joback Method
dvisc	0.0022101	Pa×s	402.84	Joback Method

dvisc	0.0008789	Pa×s	465.33	Joback Method
dvisc	0.0004348	Pa×s	527.82	Joback Method
dvisc	0.0002496	Pa×s	590.31	Joback Method
dvisc	0.0001594	Pa×s	652.80	Joback Method
dvisc	0.0001101	Pa×s	715.29	Joback Method
dvisc	0.0000807	Pa×s	777.78	Joback Method

Sources

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=U405459&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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