Glutaric acid, 2-(cyclohexyl)ethyl 3-methylbut-2-yl ester

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

InchiKey: WVNZZSDRVSDIRR-UHFFFAOYSA-N

Formula: C18H32O4

SMILES: CC(C)C(C)OC(=O)CCCC(=O)OCCC1CCCCC1

Mol. weight [g/mol]: 312.44

Physical Properties

Property code	Value	Unit	Source
gf	-347.59	kJ/mol	Joback Method
hf	-860.69	kJ/mol	Joback Method
hfus	32.74	kJ/mol	Joback Method
hvap	73.63	kJ/mol	Joback Method
log10ws	-4.61		Crippen Method
logp	4.258		Crippen Method
mcvol	268.500	ml/mol	McGowan Method
pc	1442.44	kPa	Joback Method
rinpol	2093.00		NIST Webbook
rinpol	2093.00		NIST Webbook
tb	782.49	K	Joback Method
tc	981.92	K	Joback Method
tf	414.32	K	Joback Method
vc	1.012	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	846.94	J/mol×K	782.49	Joback Method
cpg	866.02	J/mol×K	815.73	Joback Method
cpg	883.83	J/mol×K	848.97	Joback Method
cpg	900.38	J/mol×K	882.21	Joback Method
cpg	915.68	J/mol×K	915.44	Joback Method
cpg	929.77	J/mol×K	948.68	Joback Method
cpg	942.65	J/mol×K	981.92	Joback Method
dvisc	0.0017533	Pa×s	414.32	Joback Method

dvisc	0.0007016	Pa×s	475.68	Joback Method
dvisc	0.0003461	Pa×s	537.04	Joback Method
dvisc	0.0001974	Pa×s	598.40	Joback Method
dvisc	0.0001249	Pa×s	659.77	Joback Method
dvisc	0.0000855	Pa×s	721.13	Joback Method
dvisc	0.0000621	Pa×s	782.49	Joback Method

Sources

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=U405415&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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