Glutaric acid, ethyl 1-phenylpropyl ester

Inchi: InChI=1S/C16H22O4/c1-3-14(13-9-6-5-7-10-13)20-16(18)12-8-11-15(17)19-4-2/h5-7,9-1
InchiKey: LNLFMHRTUCNCDH-UHFFFAOYSA-N
Formula: C16H22O4
SMILES: CCOC(=O)CCCC(=O)OC(CC)c1ccccc1
Mol. weight [g/mol]: 278.34

Physical Properties

Property code	Value	Unit	Source
gf	-274.03	kJ/mol	Joback Method
hf	-631.92	kJ/mol	Joback Method
hfus	33.29	kJ/mol	Joback Method
hvap	71.41	kJ/mol	Joback Method
log10ws	-3.81		Crippen Method
logp	3.414		Crippen Method
mcvol	227.420	ml/mol	McGowan Method
pc	1853.11	kPa	Joback Method
rinpol	1973.00		NIST Webbook
tb	744.30	K	Joback Method
tc	948.22	K	Joback Method
tf	425.82	K	Joback Method
vc	0.866	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	649.77	J/mol×K	744.30	Joback Method
cpg	665.24	J/mol×K	778.29	Joback Method
cpg	679.68	J/mol×K	812.27	Joback Method
cpg	693.12	J/mol×K	846.26	Joback Method
cpg	705.57	J/mol×K	880.25	Joback Method
cpg	717.05	J/mol×K	914.23	Joback Method
cpg	727.58	J/mol×K	948.22	Joback Method
dvisc	0.0012005	Pa×s	425.82	Joback Method
dvisc	0.0006062	Pa×s	478.90	Joback Method

dvisc	0.0003509	Pa×s	531.98	Joback Method
dvisc	0.0002242	Pa×s	585.06	Joback Method
dvisc	0.0001544	Pa×s	638.14	Joback Method
dvisc	0.0001126	Pa×s	691.22	Joback Method
dvisc	0.0000859	Pa×s	744.30	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=U358947&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