Glutaric acid, 1-phenylpropyl propyl ester

Inchi: InChI=1S/C17H24O4/c1-3-13-20-16(18)11-8-12-17(19)21-15(4-2)14-9-6-5-7-10-14/h5-7,
InchiKey: ZDJAZZJWVAFNTF-UHFFFAOYSA-N
Formula: C17H24O4
SMILES: CCCOC(=O)CCCC(=O)OC(CC)c1ccccc1
Mol. weight [g/mol]: 292.37

Physical Properties

Property code	Value	Unit	Source
gf	-265.61	kJ/mol	Joback Method
hf	-652.56	kJ/mol	Joback Method
hfus	35.88	kJ/mol	Joback Method
hvap	73.64	kJ/mol	Joback Method
log10ws	-4.23		Crippen Method
logp	3.804		Crippen Method
mcvol	241.510	ml/mol	McGowan Method
pc	1708.95	kPa	Joback Method
rinpol	2075.00		NIST Webbook
tb	767.18	K	Joback Method
tc	969.48	K	Joback Method
tf	437.09	K	Joback Method
vc	0.921	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	705.62	J/mol×K	767.18	Joback Method
cpg	773.93	J/mol×K	935.76	Joback Method
cpg	762.30	J/mol×K	902.04	Joback Method
cpg	749.67	J/mol×K	868.33	Joback Method
cpg	736.03	J/mol×K	834.61	Joback Method
cpg	721.35	J/mol×K	800.90	Joback Method
cpg	784.60	J/mol×K	969.48	Joback Method
dvisc	0.0000752	Pa×s	767.18	Joback Method
dvisc	0.0000989	Pa×s	712.16	Joback Method

dvisc	0.0001362	Pa×s	657.15	Joback Method
dvisc	0.0001988	Pa×s	602.13	Joback Method
dvisc	0.0003130	Pa×s	547.12	Joback Method
dvisc	0.0005455	Pa×s	492.11	Joback Method
dvisc	0.0010935	Pa×s	437.09	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=U358948&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

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