Glutaric acid, di(phenethyl) ester

Inchi: InChI=1S/C21H24O4/c22-20(24-16-14-18-8-3-1-4-9-18)12-7-13-21(23)25-17-15-19-10-5
InchiKey: DQGLXZKTFZULTC-UHFFFAOYSA-N
Formula: C21H24O4
SMILES: O=C(CCCC(=O)OCCc1ccccc1)OCCc1ccccc1
Mol. weight [g/mol]: 340.41

Physical Properties

Property code	Value	Unit	Source
gf	-117.08	kJ/mol	Joback Method
hf	-493.31	kJ/mol	Joback Method
hfus	43.80	kJ/mol	Joback Method
hvap	85.20	kJ/mol	Joback Method
log10ws	-4.54		Crippen Method
logp	3.728		Crippen Method
mcvol	274.110	ml/mol	McGowan Method
pc	1625.91	kPa	Joback Method
rinpol	2792.00		NIST Webbook
tb	885.82	K	Joback Method
tc	1107.40	K	Joback Method
tf	523.59	K	Joback Method
vc	1.044	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	840.39	J/mol×K	885.82	Joback Method
cpg	854.77	J/mol×K	922.75	Joback Method
cpg	867.85	J/mol×K	959.68	Joback Method
cpg	879.70	J/mol×K	996.61	Joback Method
cpg	890.35	J/mol×K	1033.54	Joback Method
cpg	899.87	J/mol×K	1070.47	Joback Method
cpg	908.28	J/mol×K	1107.40	Joback Method
dvisc	0.0005373	Pa×s	523.59	Joback Method
dvisc	0.0002918	Pa×s	583.96	Joback Method

dvisc	0.0001777	Pa×s	644.33	Joback Method
dvisc	0.0001178	Pa×s	704.70	Joback Method
dvisc	0.0000834	Pa×s	765.08	Joback Method
dvisc	0.0000620	Pa×s	825.45	Joback Method
dvisc	0.0000481	Pa×s	885.82	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=U358694&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