Glutaric acid, hept-2-yl 3-phenylpropyl ester

Inchi: InChI=1S/C21H32O4/c1-3-4-6-11-18(2)25-21(23)16-9-15-20(22)24-17-10-14-19-12-7-5-8
InchiKey: GWSPBEVKJCMHDL-UHFFFAOYSA-N
Formula: C21H32O4
SMILES: CCCCCC(C)OC(=O)CCCC(=O)OCCCc1ccccc1
Mol. weight [g/mol]: 348.48

Physical Properties

Property code	Value	Unit	Source
gf	-231.93	kJ/mol	Joback Method
hf	-735.12	kJ/mol	Joback Method
hfus	46.24	kJ/mol	Joback Method
hvap	82.54	kJ/mol	Joback Method
log10ws	-5.55		Crippen Method
logp	4.845		Crippen Method
mcvol	297.870	ml/mol	McGowan Method
pc	1272.78	kPa	Joback Method
rinpol	2482.00		NIST Webbook
rinpol	2482.00		NIST Webbook
tb	858.70	K	Joback Method
tc	1060.45	K	Joback Method
tf	482.17	K	Joback Method
vc	1.145	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	938.24	J/mol×K	858.70	Joback Method
cpg	1009.22	J/mol×K	1026.83	Joback Method
cpg	997.29	J/mol×K	993.20	Joback Method
cpg	984.26	J/mol×K	959.58	Joback Method
cpg	970.10	J/mol×K	925.95	Joback Method
cpg	954.76	J/mol×K	892.33	Joback Method
cpg	1020.07	J/mol×K	1060.45	Joback Method
dvisc	0.0000430	Pa×s	858.70	Joback Method

dvisc	0.0000571	Pa×s	795.94	Joback Method
dvisc	0.0000797	Pa×s	733.19	Joback Method
dvisc	0.0001183	Pa×s	670.43	Joback Method
dvisc	0.0001906	Pa×s	607.68	Joback Method
dvisc	0.0003427	Pa×s	544.92	Joback Method
dvisc	0.0007178	Pa×s	482.17	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=U391774&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