Glutaric acid, cyclohexylmethyl 1-phenylpropyl ester

Inchi: InChI=1S/C21H30O4/c1-2-19(18-12-7-4-8-13-18)25-21(23)15-9-14-20(22)24-16-17-10-5

InchiKey: ZWBONTNYNHPJDS-UHFFFAOYSA-N

Formula: C21H30O4

SMILES: CCC(OC(=O)CCCC(=O)OCC1CCCCC1)c1ccccc1

Mol. weight [g/mol]: 346.46

Physical Properties

Property code	Value	Unit	Source
gf	-207.48	kJ/mol	Joback Method
hf	-680.80	kJ/mol	Joback Method
hfus	38.07	kJ/mol	Joback Method
hvap	82.97	kJ/mol	Joback Method
log10ws	-5.55		Crippen Method
logp	4.975		Crippen Method
mcvol	287.010	ml/mol	McGowan Method
pc	1481.57	kPa	Joback Method
rinpol	2540.00		NIST Webbook
rinpol	2540.00		NIST Webbook
tb	878.25	K	Joback Method
tc	1098.08	K	Joback Method
tf	489.55	K	Joback Method
vc	1.079	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	933.63	J/mol×K	878.25	Joback Method
cpg	1004.57	J/mol×K	1061.45	Joback Method
cpg	993.30	J/mol×K	1024.81	Joback Method
cpg	980.61	J/mol×K	988.17	Joback Method
cpg	966.47	J/mol×K	951.53	Joback Method
cpg	950.82	J/mol×K	914.89	Joback Method
cpg	1014.47	J/mol×K	1098.08	Joback Method
dvisc	0.0000443	Pa×s	878.25	Joback Method

dvisc	0.0000594	Pa×s	813.47	Joback Method
dvisc	0.0000836	Pa×s	748.68	Joback Method
dvisc	0.0001256	Pa×s	683.90	Joback Method
dvisc	0.0002056	Pa×s	619.12	Joback Method
dvisc	0.0003776	Pa×s	554.33	Joback Method
dvisc	0.0008144	Pa×s	489.55	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U392048&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Joback Method:	https://en.wikipedia.org/wiki/Joback_method

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