Glutaric acid, isobutyl 5-methoxy-3-phenylpentyl ester

Inchi: InChI=1S/C21H32O5/c1-17(2)16-26-21(23)11-7-10-20(22)25-15-13-19(12-14-24-3)18-8-

InchiKey: BIHRAWDWJULMGB-UHFFFAOYSA-N

Formula: C21H32O5

SMILES: COCCC(CCOC(=O)CCCC(=O)OCC(C)C)c1ccccc1

Mol. weight [g/mol]: 364.48

Physical Properties

Property code	Value	Unit	Source
gf	-339.37	kJ/mol	Joback Method
hf	-872.62	kJ/mol	Joback Method
hfus	43.90	kJ/mol	Joback Method
hvap	84.56	kJ/mol	Joback Method
log10ws	-4.25		Crippen Method
logp	4.109		Crippen Method
mcvol	303.740	ml/mol	McGowan Method
pc	1264.65	kPa	Joback Method
rinpol	2563.00		NIST Webbook
rinpol	2563.00		NIST Webbook
tb	880.68	K	Joback Method
tc	1085.58	K	Joback Method
tf	489.40	K	Joback Method
vc	1.157	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	968.39	J/mol×K	880.68	Joback Method
cpg	1035.75	J/mol×K	1051.43	Joback Method
cpg	1024.83	J/mol×K	1017.28	Joback Method
cpg	1012.65	J/mol×K	983.13	Joback Method
cpg	999.20	J/mol×K	948.98	Joback Method
cpg	984.45	J/mol×K	914.83	Joback Method
cpg	1045.42	J/mol×K	1085.58	Joback Method
dvisc	0.0000293	Pa×s	880.68	Joback Method

dvisc	0.0000394	Pa×s	815.47	Joback Method
dvisc	0.0000557	Pa×s	750.25	Joback Method
dvisc	0.0000842	Pa×s	685.04	Joback Method
dvisc	0.0001388	Pa×s	619.83	Joback Method
dvisc	0.0002575	Pa×s	554.61	Joback Method
dvisc	0.0005629	Pa×s	489.40	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U359529&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