Glutaric acid, 2,5-dimethylphenyl isobutyl ester

Inchi: InChI=1S/C17H24O4/c1-12(2)11-20-16(18)6-5-7-17(19)21-15-10-13(3)8-9-14(15)4/h8-10

InchiKey: ZRVJLRMLQLTYPF-UHFFFAOYSA-N

Formula: C17H24O4

SMILES: Cc1ccc(C)c(OC(=O)CCCC(=O)OCC(C)C)c1

Mol. weight [g/mol]: 292.37

Physical Properties

Property code	Value	Unit	Source
gf	-284.87	kJ/mol	Joback Method
hf	-675.50	kJ/mol	Joback Method
hfus	35.10	kJ/mol	Joback Method
hvap	74.96	kJ/mol	Joback Method
log10ws	-4.29		Crippen Method
logp	3.578		Crippen Method
mcvol	241.510	ml/mol	McGowan Method
pc	1667.33	kPa	Joback Method
rinpol	2128.00		NIST Webbook
rinpol	2128.00		NIST Webbook
tb	777.14	K	Joback Method
tc	981.04	K	Joback Method
tf	462.13	K	Joback Method
vc	0.921	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	704.13	J/mol×K	777.14	Joback Method
cpg	719.66	J/mol×K	811.12	Joback Method
cpg	734.15	J/mol×K	845.11	Joback Method
cpg	747.62	J/mol×K	879.09	Joback Method
cpg	760.06	J/mol×K	913.08	Joback Method
cpg	771.51	J/mol×K	947.06	Joback Method
cpg	781.95	J/mol×K	981.04	Joback Method
dvisc	0.0007546	Pa×s	462.13	Joback Method

dvisc	0.0004235	Pa×s	514.63	Joback Method
dvisc	0.0002645	Pa×s	567.13	Joback Method
dvisc	0.0001789	Pa×s	619.63	Joback Method
dvisc	0.0001287	Pa×s	672.14	Joback Method
dvisc	0.0000971	Pa×s	724.64	Joback Method
dvisc	0.0000760	Pa×s	777.14	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U358936&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