Glutaric acid, isobutyl 3-methoxybenzyl ester

Inchi: InChI=1S/C17H24O5/c1-13(2)11-21-16(18)8-5-9-17(19)22-12-14-6-4-7-15(10-14)20-3/h4
InchiKey: RKIIITZYMPYDHJ-UHFFFAOYSA-N
Formula: C17H24O5
SMILES: COc1cccc(COC(=O)CCCC(=O)OCC(C)C)c1
Mol. weight [g/mol]: 308.37

Physical Properties

Property code	Value	Unit	Source
gf	-380.24	kJ/mol	Joback Method
hf	-796.25	kJ/mol	Joback Method
hfus	36.68	kJ/mol	Joback Method
hvap	76.71	kJ/mol	Joback Method
log10ws	-3.72		Crippen Method
logp	3.108		Crippen Method
mcvol	247.380	ml/mol	McGowan Method
pc	1664.61	kPa	Joback Method
rinpol	2291.00		NIST Webbook
tb	794.58	K	Joback Method
tc	997.23	K	Joback Method
tf	471.84	K	Joback Method
vc	0.940	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	733.23	J/mol×K	794.58	Joback Method
cpg	748.43	J/mol×K	828.36	Joback Method
cpg	762.53	J/mol×K	862.13	Joback Method
cpg	775.55	J/mol×K	895.91	Joback Method
cpg	787.49	J/mol×K	929.68	Joback Method
cpg	798.35	J/mol×K	963.46	Joback Method
cpg	808.13	J/mol×K	997.23	Joback Method
dvisc	0.0006330	Pa×s	471.84	Joback Method
dvisc	0.0003456	Pa×s	525.63	Joback Method

dvisc	0.0002112	Pa×s	579.42	Joback Method
dvisc	0.0001403	Pa×s	633.21	Joback Method
dvisc	0.0000994	Pa×s	687.00	Joback Method
dvisc	0.0000740	Pa×s	740.79	Joback Method
dvisc	0.0000573	Pa×s	794.58	Joback Method

Sources

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
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U377188&Units=SI

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