Glutaric acid, 3-methylbut-2-yl 4-methoxybenzyl ester

Inchi: InChI=1S/C18H26O5/c1-13(2)14(3)23-18(20)7-5-6-17(19)22-12-15-8-10-16(21-4)11-9-15

InchiKey: MDVJBIXIERJAOP-UHFFFAOYSA-N

Formula: C18H26O5

SMILES: COc1ccc(COC(=O)CCCC(=O)OC(C)C(C)C)cc1

Mol. weight [g/mol]: 322.40

Physical Properties

Property code	Value	Unit	Source
gf	-374.26	kJ/mol	Joback Method
hf	-822.17	kJ/mol	Joback Method
hfus	35.74	kJ/mol	Joback Method
hvap	78.55	kJ/mol	Joback Method
log10ws	-4.25		Crippen Method
logp	3.496		Crippen Method
mcvol	261.470	ml/mol	McGowan Method
pc	1551.22	kPa	Joback Method
rinpol	2335.00		NIST Webbook
rinpol	2335.00		NIST Webbook
tb	817.02	K	Joback Method
tc	1021.36	K	Joback Method
tf	468.11	K	Joback Method
vc	0.990	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	791.08	J/mol×K	817.02	Joback Method
cpg	857.24	J/mol×K	987.30	Joback Method
cpg	846.33	J/mol×K	953.25	Joback Method
cpg	834.26	J/mol×K	919.19	Joback Method
cpg	821.03	J/mol×K	885.13	Joback Method
cpg	806.64	J/mol×K	851.08	Joback Method
cpg	867.00	J/mol×K	1021.36	Joback Method
dvisc	0.0000459	Pa×s	817.02	Joback Method

dvisc	0.0000603	Pa×s	758.87	Joback Method
dvisc	0.0000830	Pa×s	700.72	Joback Method
dvisc	0.0001211	Pa×s	642.57	Joback Method
dvisc	0.0001903	Pa×s	584.41	Joback Method
dvisc	0.0003307	Pa×s	526.26	Joback Method
dvisc	0.0006591	Pa×s	468.11	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U391739&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
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

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