Glutaric acid, di(5-methyl-2-methoxybenzyl) ester

Inchi: InChI=1S/C21H24O6/c1-14-8-10-16(24-3)18(12-14)26-20(22)6-5-7-21(23)27-19-13-15(2

InchiKey: MKIDKWJVEGCGSX-UHFFFAOYSA-N

Formula: C21H24O6

SMILES: COc1ccc(C)cc1OC(=O)CCCC(=O)Oc1cc(C)ccc1OC

Mol. weight [g/mol]: 372.41

Physical Properties

Property code	Value	Unit	Source
gf	-365.60	kJ/mol	Joback Method
hf	-803.63	kJ/mol	Joback Method
hfus	44.62	kJ/mol	Joback Method
hvap	92.67	kJ/mol	Joback Method
log10ws	-5.36		Crippen Method
logp	4.002		Crippen Method
mcvol	285.850	ml/mol	McGowan Method
pc	1509.33	kPa	Joback Method
rinpol	2901.00		NIST Webbook
tb	950.58	K	Joback Method
tc	1175.75	K	Joback Method
tf	618.13	K	Joback Method
vc	1.079	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	889.84	J/mol×K	950.58	Joback Method
cpg	902.04	J/mol×K	988.11	Joback Method
cpg	912.62	J/mol×K	1025.64	Joback Method
cpg	921.57	J/mol×K	1063.16	Joback Method
cpg	928.89	J/mol×K	1100.69	Joback Method
cpg	934.56	J/mol×K	1138.22	Joback Method
cpg	938.55	J/mol×K	1175.75	Joback Method
dvisc	0.0001708	Pa×s	618.13	Joback Method
dvisc	0.0001126	Pa×s	673.54	Joback Method

dvisc	0.0000791	Pa×s	728.95	Joback Method
dvisc	0.0000584	Pa×s	784.36	Joback Method
dvisc	0.0000449	Pa×s	839.76	Joback Method
dvisc	0.0000356	Pa×s	895.17	Joback Method
dvisc	0.0000291	Pa×s	950.58	Joback Method

Sources

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=U393936&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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