Glutaric acid, 2-methylpent-3-yl 5-methyl-2-methoxybenzyl ester

Inchi: InChI=1S/C19H28O5/c1-6-15(13(2)3)23-18(20)8-7-9-19(21)24-17-12-14(4)10-11-16(17)2

InchiKey: SMOYPMBVXIXJFD-UHFFFAOYSA-N

Formula: C19H28O5

SMILES: CCC(OC(=O)CCCC(=O)Oc1cc(C)ccc1OC)C(C)C

Mol. weight [g/mol]: 336.42

Physical Properties

Property code	Value	Unit	Source
gf	-375.47	kJ/mol	Joback Method
hf	-854.28	kJ/mol	Joback Method
hfus	37.95	kJ/mol	Joback Method
hvap	81.43	kJ/mol	Joback Method
log10ws	-4.88		Crippen Method
logp	4.057		Crippen Method
mcvol	275.560	ml/mol	McGowan Method
pc	1423.99	kPa	Joback Method
rinpol	2325.00		NIST Webbook
tb	844.88	K	Joback Method
tc	1049.84	K	Joback Method
tf	491.90	K	Joback Method
vc	1.046	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	848.48	J/mol×K	844.88	Joback Method
cpg	864.09	J/mol×K	879.04	Joback Method
cpg	878.49	J/mol×K	913.20	Joback Method
cpg	891.66	J/mol×K	947.36	Joback Method
cpg	903.61	J/mol×K	981.52	Joback Method
cpg	914.34	J/mol×K	1015.68	Joback Method
cpg	923.85	J/mol×K	1049.84	Joback Method
dvisc	0.0004996	Pa×s	491.90	Joback Method
dvisc	0.0002624	Pa×s	550.73	Joback Method

dvisc	0.0001561	Pa×s	609.56	Joback Method
dvisc	0.0001017	Pa×s	668.39	Joback Method
dvisc	0.0000711	Pa×s	727.22	Joback Method
dvisc	0.0000524	Pa×s	786.05	Joback Method
dvisc	0.0000403	Pa×s	844.88	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=U393922&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