Glutaric acid, ethyl 5-methoxy-3-phenylpentyl ester

Inchi: InChI=1S/C19H28O5/c1-3-23-18(20)10-7-11-19(21)24-15-13-17(12-14-22-2)16-8-5-4-6-9

InchiKey: VNGWIWCEQXRDCG-UHFFFAOYSA-N

Formula: C19H28O5

SMILES: CCOC(=O)CCCC(=O)OCCC(CCOC)c1ccccc1

Mol. weight [g/mol]: 336.42

Physical Properties

Property code	Value	Unit	Source
gf	-353.77	kJ/mol	Joback Method
hf	-826.06	kJ/mol	Joback Method
hfus	42.25	kJ/mol	Joback Method
hvap	80.50	kJ/mol	Joback Method
log10ws	-3.65		Crippen Method
logp	3.473		Crippen Method
mcvol	275.560	ml/mol	McGowan Method
pc	1447.94	kPa	Joback Method
rinpol	2404.00		NIST Webbook
tb	835.36	K	Joback Method
tc	1036.71	K	Joback Method
tf	481.86	K	Joback Method
vc	1.052	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	849.41	J/mol×K	835.36	Joback Method
cpg	865.08	J/mol×K	868.92	Joback Method
cpg	879.57	J/mol×K	902.48	Joback Method
cpg	892.90	J/mol×K	936.03	Joback Method
cpg	905.07	J/mol×K	969.59	Joback Method
cpg	916.10	J/mol×K	1003.15	Joback Method
cpg	925.99	J/mol×K	1036.71	Joback Method
dvisc	0.0006138	Pa×s	481.86	Joback Method
dvisc	0.0003094	Pa×s	540.78	Joback Method

dvisc	0.0001785	Pa×s	599.69	Joback Method
dvisc	0.0001136	Pa×s	658.61	Joback Method
dvisc	0.0000779	Pa×s	717.53	Joback Method
dvisc	0.0000565	Pa×s	776.44	Joback Method
dvisc	0.0000429	Pa×s	835.36	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=U359527&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

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