Glutaric acid, cyclohexylmethyl 2-methoxyphenyl ester

Inchi: InChI=1S/C19H26O5/c1-22-16-10-5-6-11-17(16)24-19(21)13-7-12-18(20)23-14-15-8-3-2

InchiKey: ITKLQCHKEGPKAA-UHFFFAOYSA-N

Formula: C19H26O5

SMILES: COc1ccccc1OC(=O)CCCC(=O)OCC1CCCCC1

Mol. weight [g/mol]: 334.41

Physical Properties

Property code	Value	Unit	Source
gf	-336.51	kJ/mol	Joback Method
hf	-777.93	kJ/mol	Joback Method
hfus	37.21	kJ/mol	Joback Method
hvap	81.98	kJ/mol	Joback Method
log10ws	-4.61		Crippen Method
logp	3.894		Crippen Method
mcvol	264.700	ml/mol	McGowan Method
pc	1671.43	kPa	Joback Method
rinpol	2595.00		NIST Webbook
tb	860.33	K	Joback Method
tc	1080.25	K	Joback Method
tf	516.76	K	Joback Method
vc	0.991	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	842.94	J/mol×K	860.33	Joback Method
cpg	908.88	J/mol×K	1043.60	Joback Method
cpg	898.70	J/mol×K	1006.95	Joback Method
cpg	887.03	J/mol×K	970.29	Joback Method
cpg	873.86	J/mol×K	933.64	Joback Method
cpg	859.16	J/mol×K	896.98	Joback Method
cpg	917.57	J/mol×K	1080.25	Joback Method
dvisc	0.0000490	Pa×s	860.33	Joback Method
dvisc	0.0000632	Pa×s	803.07	Joback Method

dvisc	0.0000847	Pa×s	745.81	Joback Method
dvisc	0.0001192	Pa×s	688.54	Joback Method
dvisc	0.0001785	Pa×s	631.28	Joback Method
dvisc	0.0002896	Pa×s	574.02	Joback Method
dvisc	0.0005233	Pa×s	516.76	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=U391762&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