Glutaric acid, cyclohexylmethyl 4-methoxybenzyl ester

Inchi: InChI=1S/C20H28O5/c1-23-18-12-10-17(11-13-18)15-25-20(22)9-5-8-19(21)24-14-16-6-

InchiKey: QUEOWYCKFHCFGA-UHFFFAOYSA-N

Formula: C20H28O5

SMILES: COc1ccc(COC(=O)CCCC(=O)OCC2CCCCC2)cc1

Mol. weight [g/mol]: 348.43

Physical Properties

Property code	Value	Unit	Source
gf	-328.09	kJ/mol	Joback Method
hf	-798.57	kJ/mol	Joback Method
hfus	39.80	kJ/mol	Joback Method
hvap	84.20	kJ/mol	Joback Method
log10ws	-4.87		Crippen Method
logp	4.032		Crippen Method
mcvol	278.790	ml/mol	McGowan Method
pc	1547.57	kPa	Joback Method
rinpol	2773.00		NIST Webbook
rinpol	2773.00		NIST Webbook
tb	883.21	K	Joback Method
tc	1102.01	K	Joback Method
tf	528.03	K	Joback Method
vc	1.046	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	902.00	J/mol×K	883.21	Joback Method
cpg	967.21	J/mol×K	1065.54	Joback Method
cpg	957.23	J/mol×K	1029.08	Joback Method
cpg	945.74	J/mol×K	992.61	Joback Method
cpg	932.72	J/mol×K	956.14	Joback Method
cpg	918.14	J/mol×K	919.68	Joback Method
cpg	975.68	J/mol×K	1102.01	Joback Method
dvisc	0.0000425	Pa×s	883.21	Joback Method

dvisc	0.0000549	Pa×s	824.01	Joback Method
dvisc	0.0000738	Pa×s	764.82	Joback Method
dvisc	0.0001044	Pa×s	705.62	Joback Method
dvisc	0.0001573	Pa×s	646.42	Joback Method
dvisc	0.0002575	Pa×s	587.23	Joback Method
dvisc	0.0004706	Pa×s	528.03	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U391744&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