Glutaric acid, cyclohexylmethyl 2,6-dimethoxyphenyl ester

Inchi: InChI=1S/C20H28O6/c1-23-16-10-6-11-17(24-2)20(16)26-19(22)13-7-12-18(21)25-14-15

InchiKey: DWOZDGVHLLOFOA-UHFFFAOYSA-N

Formula: C20H28O6

SMILES: COc1cccc(OC)c1OC(=O)CCCC(=O)OCC1CCCCC1

Mol. weight [g/mol]: 364.43

Physical Properties

Property code	Value	Unit	Source
gf	-442.72	kJ/mol	Joback Method
hf	-942.26	kJ/mol	Joback Method
hfus	40.60	kJ/mol	Joback Method
hvap	87.27	kJ/mol	Joback Method
log10ws	-4.73		Crippen Method
logp	3.903		Crippen Method
mcvol	284.660	ml/mol	McGowan Method
pc	1509.33	kPa	Joback Method
rinpol	2782.00		NIST Webbook
rinpol	2782.00		NIST Webbook
tb	910.61	K	Joback Method
tc	1130.33	K	Joback Method
tf	562.78	K	Joback Method
vc	1.065	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	929.82	J/mol×K	910.61	Joback Method
cpg	944.90	J/mol×K	947.23	Joback Method
cpg	958.29	J/mol×K	983.85	Joback Method
cpg	969.98	J/mol×K	1020.47	Joback Method
cpg	979.95	J/mol×K	1057.09	Joback Method
cpg	988.21	J/mol×K	1093.71	Joback Method
cpg	994.74	J/mol×K	1130.33	Joback Method
dvisc	0.0002881	Pa×s	562.78	Joback Method

dvisc	0.0001686	Pa×s	620.75	Joback Method
dvisc	0.0001081	Pa×s	678.72	Joback Method
dvisc	0.0000743	Pa×s	736.69	Joback Method
dvisc	0.0000540	Pa×s	794.67	Joback Method
dvisc	0.0000410	Pa×s	852.64	Joback Method
dvisc	0.0000322	Pa×s	910.61	Joback Method

Sources

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=U392007&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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