Glutaric acid, hept-2-yl 2,6-dimethoxyphenyl ester

Inchi: InChI=1S/C20H30O6/c1-5-6-7-10-15(2)25-18(21)13-9-14-19(22)26-20-16(23-3)11-8-12-1

InchiKey: QJJZENZNYPRMAT-UHFFFAOYSA-N

Formula: C20H30O6

SMILES: CCCCCC(C)OC(=O)CCCC(=O)Oc1c(OC)cccc1OC

Mol. weight [g/mol]: 366.45

Physical Properties

Property code	Value	Unit	Source
gf	-469.61	kJ/mol	Joback Method
hf	-1001.86	kJ/mol	Joback Method
hfus	45.25	kJ/mol	Joback Method
hvap	86.46	kJ/mol	Joback Method
log10ws	-5.19		Crippen Method
logp	4.291		Crippen Method
mcvol	295.520	ml/mol	McGowan Method
pc	1302.35	kPa	Joback Method
rinpol	2542.00		NIST Webbook
rinpol	2542.00		NIST Webbook
tb	890.62	K	Joback Method
tc	1096.34	K	Joback Method
tf	540.40	K	Joback Method
vc	1.125	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	935.91	J/mol×K	890.62	Joback Method
cpg	950.95	J/mol×K	924.91	Joback Method
cpg	964.63	J/mol×K	959.19	Joback Method
cpg	976.93	J/mol×K	993.48	Joback Method
cpg	987.85	J/mol×K	1027.77	Joback Method
cpg	997.38	J/mol×K	1062.05	Joback Method
cpg	1005.51	J/mol×K	1096.34	Joback Method
dvisc	0.0002808	Pa×s	540.40	Joback Method

dvisc	0.0001593	Pa×s	598.77	Joback Method
dvisc	0.0000999	Pa×s	657.14	Joback Method
dvisc	0.0000676	Pa×s	715.51	Joback Method
dvisc	0.0000486	Pa×s	773.88	Joback Method
dvisc	0.0000365	Pa×s	832.25	Joback Method
dvisc	0.0000285	Pa×s	890.62	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U392004&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