Glutaric acid, 8-chlorooctyl 2,6-dimethoxyphenyl ester

Inchi: InChI=1S/C21H31ClO6/c1-25-17-11-9-12-18(26-2)21(17)28-20(24)14-10-13-19(23)27-16

InchiKey: PGSCOAIZQAJRJI-UHFFFAOYSA-N

Formula: C21H31ClO6

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

Mol. weight [g/mol]: 414.92

Physical Properties

Property code	Value	Unit	Source
gf	-470.68	kJ/mol	Joback Method
hf	-1032.96	kJ/mol	Joback Method
hfus	55.56	kJ/mol	Joback Method
hvap	93.46	kJ/mol	Joback Method
log10ws	-5.65		Crippen Method
logp	4.902		Crippen Method
mcvol	321.850	ml/mol	McGowan Method
pc	1179.28	kPa	Joback Method
rinpol	3075.00		NIST Webbook
tb	951.37	K	Joback Method
tc	1165.65	K	Joback Method
tf	596.59	K	Joback Method
vc	1.236	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1020.12	J/mol×K	951.37	Joback Method
cpg	1033.85	J/mol×K	987.08	Joback Method
cpg	1046.06	J/mol×K	1022.80	Joback Method
cpg	1056.75	J/mol×K	1058.51	Joback Method
cpg	1065.91	J/mol×K	1094.22	Joback Method
cpg	1073.54	J/mol×K	1129.94	Joback Method
cpg	1079.64	J/mol×K	1165.65	Joback Method
dvisc	0.0001880	Pa×s	596.59	Joback Method
dvisc	0.0001130	Pa×s	655.72	Joback Method

dvisc	0.0000738	Pa×s	714.85	Joback Method
dvisc	0.0000515	Pa×s	773.98	Joback Method
dvisc	0.0000378	Pa×s	833.11	Joback Method
dvisc	0.0000289	Pa×s	892.24	Joback Method
dvisc	0.0000229	Pa×s	951.37	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=U392010&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