Glutaric acid, 8-chlorooctyl 3-phenylpropyl ester

Inchi: InChI=1S/C22H33ClO4/c23-17-8-3-1-2-4-9-18-26-21(24)15-10-16-22(25)27-19-11-14-20
InchiKey: RHZFTOHMWLVXAS-UHFFFAOYSA-N
Formula: C22H33ClO4
SMILES: O=C(CCCC(=O)OCCCc1ccccc1)OCCCCCCCCCl
Mol. weight [g/mol]: 396.95

Physical Properties

Property code	Value	Unit	Source
gf	-233.00	kJ/mol	Joback Method
hf	-766.22	kJ/mol	Joback Method
hfus	56.55	kJ/mol	Joback Method
hvap	89.54	kJ/mol	Joback Method
log10ws	-6.01		Crippen Method
logp	5.455		Crippen Method
mcvol	324.200	ml/mol	McGowan Method
pc	1153.78	kPa	Joback Method
rinpol	3047.00		NIST Webbook
rinpol	3047.00		NIST Webbook
tb	919.45	K	Joback Method
tc	1128.16	K	Joback Method
tf	538.36	K	Joback Method
vc	1.256	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1025.13	J/mol×K	919.45	Joback Method
cpg	1040.62	J/mol×K	954.23	Joback Method
cpg	1054.87	J/mol×K	989.02	Joback Method
cpg	1067.91	J/mol×K	1023.80	Joback Method
cpg	1079.79	J/mol×K	1058.59	Joback Method
cpg	1090.53	J/mol×K	1093.37	Joback Method
cpg	1100.20	J/mol×K	1128.16	Joback Method
dvisc	0.0004460	Pa×s	538.36	Joback Method

dvisc	0.0002325	Pa×s	601.88	Joback Method
dvisc	0.0001372	Pa×s	665.39	Joback Method
dvisc	0.0000888	Pa×s	728.90	Joback Method
dvisc	0.0000616	Pa×s	792.42	Joback Method
dvisc	0.0000451	Pa×s	855.93	Joback Method
dvisc	0.0000345	Pa×s	919.45	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=U391782&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